



Modelling and control of an activated sludge process using ASM2d and taking into account sludge floc distribution effects

PhD Thesis

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This thesis is submitted in partial fulfilment of the requirements for
the degree of Doctor of Philosophy

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Declaration

I declare that the work described in this thesis was originally performed by me. It is submitted in partial fulfilment of the requirements of the degree of Doctor of Philosophy at De Montfort University and has not been previously submitted for any other award in this university or any other university or college of advanced education.

Aboajela Kajaman

Dedication

This project is dedicated to those who have always

loved,

encouraged,

guided,

and supported me throughout my study.

Acknowledgements

It is a great honour to have this opportunity to dedicate my appreciation and acknowledge the contribution of supporters who have helped me to write this PhD thesis.

First and foremost, I offer my thanks and humble words of praise to ALLAH for all his blessings and guidance.

Next, I wish to extend my special and heartfelt appreciation to my Supervisor, Prof. Bogumil Ulanicki, without him this thesis would not have been possible. I have benefited greatly from his experience, wisdom and knowledge and I am proud to say that I conducted my PhD under his guiding supervision. I would also like to thank Prof. Katherine Huddersman for her valuable comments and guidance.

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My love and life to my parents, I am indebted to them both for making me standing tall today because of their advice and prayers.

Abstract

To reduce energy consumption, and to achieve the desired denitrification, the activated sludge process sometimes needs to operate at low dissolved oxygen concentrations. The ASM2d model describes the activated sludge process, if nitrification and denitrification occur during different phases in a sequencing batch reactor (SBR). Despite the widespread study of enhanced biological phosphorous removal, comprehensive sludge floc distribution model remains lacking that would better describe this process. Consequently, the integrated system model has been developed to understand the impact of floc at low DO concentrations, and during the process of biological nitrogen and phosphorous removal. In a wastewater treatment plant used in this study, the dissolved oxygen was controlled at a low concentration, $1.7gO_2m^{-3}$, and the dispersion coefficient into the floc was found to be $D = 1.2 \times 10^{-4} m^2/day$. Introduction of a number of effectiveness factors contributed to the development of the ASM2d model described herein. This developed model could be valuable for predicting process behaviours applicable under various configurations. Moreover, parameters and effectiveness factors for the model could be calibrated using a genetic algorithm approach. Optimisation was then achieved by controlling the solids retention time during the activated sludge process.

Contents

Dedication	III
Acknowledgements	IV
Abstract	V
List of Figures	X
List of Tables.....	XII
List of Abbreviations.....	XIII
1. INTRODUCTION	1
1.1 Background to project	1
1.2 Aims and objectives	3
1.3 Contributions	5
1.4 Thesis plan.....	7
2. THEORY AND LITERATURE REVIEW	10
2.1 Wastewater treatment theory.....	10
2.1.1 Issues with nitrification and denitrification.....	10
2.1.2 Biological nitrogen removal processes.....	13
2.1.3 Biological phosphorous removal.....	15
2.1.4 Biologically induced phosphate precipitation	18
2.1.5 Sequencing batch reactor (SBR)	19
- Stage 1: Filling	21
- Stage 2: Reaction.....	21
- Stage 3: Settling.....	21
- Stage 4: Decanting (Draw)	22
- Stage 5: Idling	22
2.2 WWTP operation and control	24
2.2.1 Biological Growth Kinetics.....	24

2.2.2	Effect of Sludge Retention Time (SRT).....	25
2.2.3	Effect of Temperature pH extension.....	26
2.2.4	Sludge Wasting in SBRs	27
2.2.5	Effects of SBR Cycles	28
2.3	Model of wastewater treatment process	31
2.3.1	Modelling Nitrogen Removal.....	31
2.3.2	Modelling Phosphorous Removal	32
2.3.3	Modelling Prefermentation.....	33
2.4	Process optimisation	35
2.4.1	Orthogonal collocation method	35
2.4.2	Genetic algorithms	36
2.4.3	Genetic algorithm approach	37
2.4.4	Typical characteristics of genetic algorithms	37
2.4.5	Genetic Algorithm Operators.....	38
2.5	Literature review of state-of-the-art of ASM modelling.....	41
2.5.1	Standard Model for Activated Sludge Processes.....	41
-	ASM1	42
-	UCTPHO model	43
-	ASM2	44
-	Activated Sludge Model no. 2d (ASM2d).....	45
-	Barker and Dold Prototype.....	46
-	ASM3 with Bio-P Module	46
2.5.2	State-of-the-art in removal of biological phosphorous.....	48
2.5.3	Sequence batch reactors	52
2.5.4	Activated sludge floc processes	54
3.	METHODOLOGY AND MODEL IMPLEMENTATION	56

3.1	Methodology	56
3.1.1	Mathematical Models	56
3.1.2	Solving Non-linear Equations.....	57
3.1.3	SIMBA software	58
3.1.4	Installation characteristics.....	59
-	Wastewater	59
-	Reactor operation	59
3.1.5	Simulated systems.....	61
3.1.6	Simulation Model	62
3.2	Extension of ASM2d with the floc model	63
3.2.1	Limitations and proposed modification for ASM2d.....	63
3.2.2	Model components.....	64
3.2.3	Matrix structure.....	66
3.2.4	Pathways interaction components.....	68
3.3	Flocculation.....	70
3.3.1	Introduction.....	70
3.3.2	Flocculation mechanisms.....	72
3.3.3	Aggregation and bioflocculation	74
3.3.4	Floc formation and single floc size	75
3.3.5	Mathematical equations of oxygen gradient within a single floc	77
4.	CALCULATIONS AND RESULTS	83
4.1	Analytical solutions of non-linear equations.....	83
4.1.1.	Effectiveness factors of a single floc	85
4.1.2.	Overall effectiveness factors.....	86
4.2	Operating conditions	86
4.3	Results.....	88

4.4	Discussion	90
5.	CALIBRATION PROCEDURE AND SIMULATION ANALYSIS	96
5.1	Calibration process.....	96
5.2	Genetic Algorithm Approach.....	97
5.3	Floc model calibration.....	98
5.3.1	Parameters Estimation	98
5.3.2	Floc calibration results.....	99
-	GA results.....	99
-	Correlation results	100
5.4	Calibration of ASM2d parameters	103
5.4.1	ASM2d calibration and validation.....	104
6.	SLUDGE ACCESS OPTIMISATION	110
6.1	Introduction.....	110
6.2	Solids retention time (SRT)	112
6.3	SBR control.....	112
6.4	Impact of SRT.....	113
6.5	Results and discussion	114
6.5.1	Sludge access every cycle.....	115
6.5.2	Sludge access every day	118
6.5.3	Sludge access every 2 days.....	120
7.	CONCLUSION AND FUTURE WORK.....	123
7.1	Conclusion and Summary	123
7.2	Summary of outputs and achievements.....	124
7.3	Future follow-on work	126
	Appendix	129
	References	136

List of Figures

Figure 2.1: Nitrogen transformations (Sedlak, 1991)	14
Figure 2.2: Principle of biological phosphors removal. (Adapted from Chai, 2008).	17
Figure 2.3: Phosphate accumulation by the EBPR process (Arvin, 1983)	18
Figure 2.4: The order of events in the sequencing batch reactor (SBR)	20
Figure 2.5: SBR for the removal of nitrogen and phosphorous	23
Figure 2.6: The biological growth cycle	24
Figure 2.7: Variation of soluble BOD and phosphorous concentration.....	29
Figure 2.8: Ammonia, Nitrate and COD concentration behaviour during SBR phases.	30
Figure 2.9: Nitrogen removal	31
Figure 2.10: Phosphorous removal	32
Figure 2.11: Fermentation model	34
Figure 2.12: Flow chart of genetic algorithm process.....	38
Figure 2.13: Figure Illustration of crossover in a binary GA.....	39
Figure 2.14: Development of the biokinetic model for an activated sludge system.	48
Figure 2.15: Schematic representation of an activated sludge floc.....	54
Figure 3.1: SIMBA control window and block library	58
Figure 3.2: Schematic representation of the laboratory apparatus	60
Figure 3.3: SBR cycle definition during one period (8 hours).....	60
Figure 3.4: Structure of a SBR with ASM2d model	61
Figure 3.5: SIMULINK system construction of SBR with ASM2d model.	62
Figure 3.6: Pathway of non-poly-P heterotrophs	68
Figure 3.7: Pathway of poly-P heterotrophs	69
Figure 3.8: Pathway of autotrophs	69
Figure 3.9: The main biological stage of the activated sludge system.....	70
Figure 3.10: Diagram of an activated sludge floc	76
Figure 3.11: A differential element of a spherical pellet	78
Figure 3.12: Pathway of hydrolysis and fermentation	81
Figure 4.1: Dissolved oxygen	89
Figure 4.2: Typical cycle response during 1 st period	89

Figure 4.3: Ammonia concentration SNH_4	90
Figure 4.4: Nitrate plus nitrite nitrogen concentration (SN_3)	91
Figure 4.5: Soluble phosphorous concentrations (orthophosphates)	92
Figure 4.6: Total Phosphorous concentration TP.....	93
Figure 4.7: Total Kjeldahl Nitrogen concentrations TKN	94
Figure 4.8: Mixed-Liquor Suspended Solids concentrations MLSS	95
Figure 5.1: Fitness value of GA versus the generation number for the floc model calibration	99
Figure 5.2: Correlation coefficient and ammonia concentration curve of (floc factors calibration).	100
Figure 5.3: Correlation and concentration curve of nitrate plus nitrite nitrogen (floc factors calibration).	101
Figure 5.4: Correlation and concentration curve of phosphorous (floc factors calibration).	102
Figure 5.5: Fitness value of GA versus generation number for ASM2d model calibration	105
Figure 5.6: Correlation coefficient and ammonia concentration curve (ASM2d model calibration).	108
Figure 5.7: Correlation coefficient and phosphorous concentration curve (ASM2d model calibration).	109
Figure 5.8: Correlation and concentration curve of nitrate plus nitrite nitrogen (ASM2d model calibration).	109
Figure 6.1: Efficiency of phosphors removal (sludge wasted every cycle)	116
Figure 6.2: Efficiency of ammonia removal (sludge wasted every cycle).....	117
Figure 6.3: MLSS concentration (sludge wasted every cycle)	117
Figure 6.4: Efficiency of phosphors removal (sludge wasted every day).....	118
Figure 6.5: Efficiency of ammonia removal (sludge wasted every day)	119
Figure 6.6: MLSS concentration (sludge wasted every cycle)	119
Figure 6.7: Efficiency of phosphors removal (sludge wasted every day).....	120
Figure 6.8: Efficiency of ammonia removal (sludge wasted every day)	121
Figure 6.9: MLSS concentration (sludge wasted every cycle)	121
Figure 7.1: The MPC block diagram.....	127

List of Tables

Table 2.1: Principle organism groups for activated sludge system.....	51
Table 3.1: Activated sludge model ASM2d components (Henze et al., 1999).....	65
Table 3.2: Process kinetics and stoichiometry for heterotrophic bacterial growth	66
Table 4.1: Distribution of flocs with different radiuses	87
Table 4.2: Assumed operating conditions	87
Table 4.3: The spread of oxygen within different floc sizes.....	88
Table 5.1: Calibration results for effectiveness floc factors	100
Table 5.2: Values of stoichiometric and kinetic parameters	104
Table 5.3: ASM2d calibration results	106
Table 6.1: Ammonia removal efficiency	114
Table 6.2: Phosphors removal efficiency	115
Table A1: Conversation factors of ASM2d	129
Table A2: ASM2d Stoichiometric Coefficients	130
Table A3: ASM2d Kinetic parameters.....	131
Table A4: Process rate equations for ASM2d.....	133
Table A5: Stoichiometric matrix.....	134

List of Abbreviations

ASM	Activated Sludge Model
ASM1	Activated Sludge Model No.1
ASM2	Activated Sludge Model No.2
ASM3	Activated Sludge Model No.3
ASP	Activated Sludge Process
BEPR	Biological enhanced phosphorous removal
BNR	Biological nutrient removal
BOD	soluble biological oxygen demand (<i>mg COD/l</i>)
COD	chemical oxygen demand (<i>mg COD/l</i>)
DAE	Differential Algebraic Equation
DNPAOs	Denitrifying Phosphorous-Accumulating Organisms
DO	Dissolved Oxygen
EBPR	Enhanced Biological Phosphorous Removal
EPS	Extracellular Polymeric Substances
EPS	extracellular polymeric substances
ESS	effluent suspended solids
HRT	Hydraulic Retention Time
IAWPRC	International Association on Water Pollution Research and Control
IAWQ	International Association on Water Quality
IWA	International Water Association

MLSS	Mixed-Liquor Suspended Solids (mg/l)
MLVSS	Mixed liquor volatile suspended solids (mg/l)
MPC	Model Predictive Control
ODE	Ordinary Deferential Equation
PAO	Phosphorous Accumulating Organisms ($mg\ P/l$)
PDE	Partial Deferential Equation
PDEs	Partial Deferential Equations
RAS	return activated-sludge
SRT	Solids Retention Time (d)
SS	Suspended Solids
SVI	Sludge Volume Index (m^3)
TKN	Total Kjeldahl Nitrogen ($mg\ N/l$)
TN	Total Nitrogen ($mg\ N/l$)
TP	Total Phosphorous ($mg\ P/l$)
VFAs	Volatile fatty acids
WWTP	Wastewater Treatment Plant

CHAPTER 1

1. INTRODUCTION

1.1 Background to project

The activated sludge process is one of the most extensively used biological wastewater treatments, and it has been modified to include different combinations of processes. It has often been instrumental in supporting a considerable expansion in capabilities to remove a variety of elements. Activated sludge models (ASMs) have been successfully used to effect intersections between WWTP plans and modelling controls, and other additional process. ASMs are also responsible for predicting biological processes performance.

A number of factors influence the physiology of sludge. Some of these include environmental conditions, operating conditions, and reactor configuration. In regard to this, the activated-sludge floc in a bioreactor, normally regarded as the influence of floc, comprises one of the most critical phenomena in the treatment and physiology of a microbial community.

While the ASM has successfully effected biological nutrient removal in many wastewater treatment plants, where nitrification and denitrification have occurred at different phases or in aerobic and anoxic tanks respectively, it needs to be enhanced through incorporation of the floc effect. This will enable denitrification in a single aeration tank in which aerobic and anoxic zones co-exist (Wang et al., 2007).

The process of the construction of microbial structures in the presence of a carbon source, and the relationship between the practical conditions in the system, has influenced microbiological studies over time.

The poor P-uptake by phosphorous accumulating organisms (PAO) can thoroughly explain the deteriorating phenomena of phosphorous removal, based on Furumai et al.'s (1999) simulated results. It seems apparent, that filament backbones can increase the floc strength, primarily at low sludge ages, while also being able to form larger aggregates and sweep fine material at high sludge ages (Eriksson et al., 1992).

Several years previously, engineers typically conducted optimisations of individual components of the system, instead of the overall system. The tendency in design has been toward the most effective unit processes while observing target efficiency, and then integrating single units to an overall optimum system of wastewater treatment. The separate minimisation of individual units in an optimal overall system is impossible, as they are part of the entire system. For an optimal solution to be accurate, accuracy must be observed in the mathematical model that describes the treatment plant operations; that is, the algorithm used in the optimisation, as well as the objective functions.

The occurrence of both nitrification and denitrification in a sequence batch reactor is termed a simultaneous process. The existence in the reactor, of aerobic and anaerobic zones with low DO concentrations, is contingent on mixing conditions, as well as aeration. Therefore, reduced rates of nitrification and denitrification occur as a result of DO effects. However, the efficiency of nutrient removal can be improved if SRT is sufficient.

1.2 Aims and objectives

Prior to specifying the particular research aims of this original study, certain fundamental questions need to be posited:

How to incorporate the sludge floc effects into an ASM2d model and how this model impacts on nitrogen and phosphorous removal?

Although the main thrust of this original research seeks to address the above question, a series of sub-questions will need to be answered in order to deal fully with this subject.

Knowledge regarding molecular phenomena related to natural aggregation remains somewhat limited. Thus, it is critical in this original research, to identify microbiological-based approaches, which can be employed to study the effects that sludge flocs have on biological phosphorous, as well as nitrogen removal.

Theoretically, two processes can be utilised in P removal. The first involves treating the oxygen only as a final electron acceptor under anaerobic-aerobic sequencing (aerobic PAOs) (Von Sperling, 2007). The second involves accumulating P, by using nitrate/nitrite as the electron acceptor, instead of oxygen; this involves denitrifying P-accumulating organisms (DNPAOs).

The Activated Sludge Model No. 2d (ASM2d) has been successfully applied to simulate nitrogen and phosphorous removal. This model was the first to consider the inhibition of the aerobic storage of polyphosphate (X_{PP}), and the aerobic growth of internal cell storage product (PHA) by PAOs (X_{PHA}); both of which affect the growth of PAOs (X_{PAO}) in the presence of COD and oxygen.

DO concentrations in the activated sludge process is usually approx. 2 mg/L, to enable organisms to grow at their maximum rate, because half-saturation constants values are intrinsic values. Therefore, most of the matters pertaining to the concentration of DO in activated sludge systems are perplexing, because the actual concentration of DO in the activated-sludge floc is not represented in the concentrations measured in the bulk liquid.

Despite the availability of all operating conditions, difficulties still exist because the concentration of DO in the bulk is not same as within the biological floc where oxygen consumption occurs. Thus, to ensure the desired growth process, it is essential to identify the amount of sludge wasted. Controlling the solids retention time (SRT) is one way to achieve this.

The objectives of this thesis can be broken down into answering the following questions:

- How can the ASM2d model be extended by creating the effectiveness floc coefficients and its dynamic behaviour is examined considering floc size distribution?
- Is it possible to develop an automatic innovative technique that can be used in the calibration of the modified ASM2d model's floc parameters to facilitate determination of whether the resultant model has the potential to achieve specific performance requirements?
- Can the significance of the floc effects on the system dynamics be evaluated?
Are the results of the simulations in-line with experimental data?

- Is it possible to optimise this modified activated sludge process by controlling the SRT and the amount of sludge access?

1.3 Contributions

In diverse situations, in which treatment plants are unable to perform the required treatments, a SBR system can be utilised to carry out the process, depending on operating conditions and the specifications of wastewater treatment. This is because of the flexibility of a SBR system for the treatment of flows, using anaerobic, aerobic and anoxic conditions in the same tank, as well as the efficiency of nutrient removal.

Although, nutrient (nitrogen and phosphorous) removal treatment is seen as an effective process in a wastewater system, it is more complicated than conventional activated sludge treatments. The unique simulation model developed and used in this original research study is based on the ASM2d, which was successfully applied in simulations of nitrogen and phosphorous removal. This unique model's system performance could be affected by many factors, such as influent wastewater characteristics, dissolved oxygen concentrations, and sludge floc size distribution.

Collocation points are an appropriate technique used in a chemical engineering environment. They are used here to calculate the spread of oxygen within a single floc. However, the novel equations developed in this original study are complicated, and it is necessary to consider using a numerical method to solve them. Thus, the orthogonal

collocation and Newton-Raphson Method were used in this original study to calculate the dissolved oxygen concentrations along the radius of the floc.

With regard to the influent and effluent flow rates, the processing time spent must be fixed under each environmental condition to be achieved; however, the sludge volume access can achieve this same result in a batch reactor system.

Accordingly, the main and original contributions of this work to this specialist area of research are:

- Studying whether a modified ASM2d with floc model could biologically enhance the process of nitrogen and phosphorous removal beyond the default model, by introducing floc related effectiveness factors. An SBR system was used in this unique research work to calibrate and validate this novel integrated model. Carvalho et al. (2007) found that a variety of PAO cells have unlike behaviours and are, consequently, able to exploit nitrate as an electron acceptor. Nevertheless, it is hypothesised that the activated sludge floc relates to PAOs that use nitrite (not nitrate).
- Calculating the effectiveness floc factors numerically, by applying the orthogonal collocation and Newton-Raphson method to the unique process equations under the operating conditions of a SBR.
- Utilising a computer-based automatic technique to estimate effectiveness and floc factors by performing a model calibration against measurements. The purpose of this technique is to minimise the fitness function using the Genetic Algorithm (GA) approach.

- Calibrating the stoichiometric and kinetic parameters for phosphorous accumulating organisms (PAOs), using GA-based approaches.
- Optimising activated sludge access and examining the effect of SRT, in terms of using different times for sludge wastage according to the dynamic removal behaviour.

1.4 Thesis plan

Chapter 2 presents the theoretical background to this study and the literature review. It provides an overview of principles relevant to the biological process of wastewater treatment. It gives a brief history of wastewater treatment theory which introduces nitrification and denitrification problems, biological phosphorous removal and sequencing batch reactor (SBR). In WWTP operation and control, biological growth kinetics effect of sludge retention time (SRT) and effect of temperature pH is presented. It also introduces the numerical application (orthogonal collocation method) used to solve model equations, and genetic algorithms (GA) for model calibration. In addition, the chapter presents a literature review which shows the standard model for activated sludge processing: the ASM1; the University of Cape Town model UCTPHO; ASM2, ASM2d, Barker and Dold Prototype, ASM3, and the Bio-P Module.

Chapter 3 encompasses the methodology used, and the model implementation. The Methodology presents the mathematical models, solves non-linear equations and describes the SIMBA software utilised for this project. The installation characteristics,

wastewater characteristics, reactor operations, simulated systems and simulation models have all been identified and defined. Moreover, it explains the key and novel research contributions of this unique study; which is the extension of ASM2d with the floc model. Initially, limitations and proposed modifications for ASM2d are described, as are the model components and matrix structure of ASM2d. In addition, the Pathways interactions of ASM2d components are shown in this section. This chapter gives a background to flocculation, presenting the flocculation mechanisms, and aggregation and bioflocculation. It also provides a detailed explanation of floc formation in connection with single floc size, and mathematical equations for the oxygen gradient within a single floc. Finally, effectiveness factors associated with a single floc are explained under the hypothetical floc model.

Chapter 4 shows the calculations and results of model simulations. These calculations are analytical solutions for non-linear equations, effectiveness factors regarding a single floc, and the overall effectiveness factors. Finally, analytical results and discussions are analysed in this chapter against the experimental data set.

Chapter 5 reviews the calibration procedure and simulation analysis. The contribution of the calibration process consists of a floc model calibration and the calibration of ASM2d parameters. In the floc model calibration, the parameters estimation and floc calibration results (GA and correlation results) are discussed. However, in the ASM2d calibration, the discussion focuses on the calibrated ASM2d parameters.

Chapter 6 outlines optimisation of sludge access in an SBR reactor, with respect to SRT, and activated sludge wasted. The results and discussion examine the biological

removal of phosphorous and nitrogen across three stages of sludge access; sludge access every cycle, sludge access every day, and sludge access every 2 days.

Chapter 7 concludes the original work presented in this thesis, and provides some suggestions for future follow-on work.

CHAPTER 2

2. THEORY AND LITERATURE REVIEW

2.1 Wastewater treatment theory

2.1.1 Issues with nitrification and denitrification

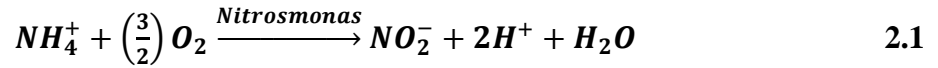
The main part in WWT is an aeration stage which is an essential part in the activated sludge process, which enables microorganisms to provide enough oxygen to allow sufficient electron acceptor capacity for metabolism. This mechanism directly affects the N and P removal, due to oxygen demand in the aeration tank. If denitrifying phosphorous removal cannot be carried out, then nitrite/nitrate should conduct the process, acting as a terminal electron acceptor under anaerobic conditions (i.e. anoxic conditions), enabling both N and P to be removed simultaneously. Although nitrate can be removed almost completely, within a short time, before the end of the filling phase via denitrification because of the plentiful carbon source, denitrifying phosphorous uptake can be executed by nitrate, which is not entirely reduced with some nitrate deposits remaining in the anaerobic phase.

The formation of an activated sludge process requires establishment of a high concentration of microorganisms (mostly bacteria; but potentially also protozoa and fungi) to eradicate any organic matter from the wastewater (Love, 1999). Nitrification and denitrification are the major processes involved in the removal of organic material.

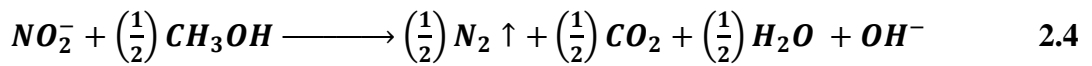
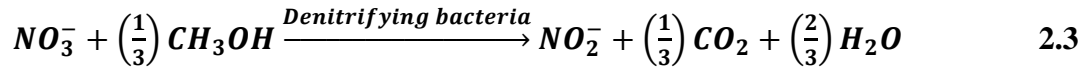
Transient conditions and steady-state conditions are two factors that can lead the relationships between DO concentration and nitrification to differ drastically. This is because of mass-transport resistance and heterotrophic competition for DO (Stenstrom and Song, 1991).

One of the most commonly applied processes, used in biological wastewater treatment, involves activated sludge and the concentration of dissolved oxygen DO levels in aerobic reactors, and has a considerable influence on the activity of heterotrophic and autotrophic microorganisms present in the activated sludge. Although, DO is usually high in the aeration tank, to degrade the organics and perform nitrification, the concentration of DO can be low, to avoid increasing energy consumption, and to achieve the desired amount of nitrogen removal during the denitrification phase.

In terms of nitrogen removal, this can be achieved in different ways; one of the commonest is bacterial nitrification, followed by bacterial denitrification.



After nitrification has been performed, the denitrification process can be applied, as in Equations 2.1 and 2.2, to convert organic N finally to N_2 gas.



The denitrification process can be repressed if the concentration of dissolved oxygen is too high; thus, the affected accumulation of nitrates and nitrogen will decrease. Moreover, when the DO concentration is too low, this can affect the nitrification leading

to insufficient nitrate availability for denitrification. Therefore, DO concentrations should be controlled, to ensure maximum nitrate production via nitrification, which can then be converted to nitrogen by denitrification.

With regard to phosphorous removal, the amount of phosphorous in the sludge depends on the amount of biochemical oxygen demand (BOD) in the anaerobic phase, as a result of denitrification of the nitrate created in the aerobic phase, as well as phosphate in the effluent and the volume of sludge produced. Conventionally, during BOD removal, phosphorous can be removed from the wastewater and converted to bacterial mass (JDB Tisis_Vanrolleghem et al., 1999).

Extensive nitrification can result in denitrification. In this case, the bacteria in the activated sludge floc use nitrate for respiration, when there is a scarcity of oxygen; thereby releasing nitrogen gas as a by-product. Since this gas has a slight solubility in water, bubbles start to form in the activated sludge, leading to the formation of a sludge blanket flotation in the final clarifier. The problem of denitrification is more hostile in the presence of a filamentous sludge, as it leads to the more extensive entrapment of nitrogen gas bubbles (Eberl, 2006).

Denitrification can only be controlled by managing the process of nitrification (minimising the aeration or age of the sludge); through the faster removal of the sludge in the final clarifier, by augmenting the concentration of dissolved oxygen in the final clarifier.

Problems associated with nitrification and denitrification are specifically burdensome in industrial waste systems, where there is ammonia supplementation. In such situations, an aeration basin must have inorganic nitrogen (ammonia or nitrate) at all times to

facilitate proper treatment, and to prevent bulking of filaments or slime. However, inorganic nitrogen should not exceed 5 mg/L, as this would lead to the development of nitrification-denitrification problems (floating sludge and low pH) (Michal, 2013).

A low pH of up to 6, which occurs as a result of extensive nitrification and low alkalinity in the wastewater, is a huge problem in some plants, as it leads to high effluent turbidity and pin floc.

2.1.2 Biological nitrogen removal processes

To more fully comprehend the amount of nitrogen present in wastewater discharges and receiving waters, four types of nitrogen should be taken into account; i.e. organic nitrogen (N_{org}), nitrite nitrogen ($NO_2^- - N$), nitrate nitrogen ($NO_3^- - N$), and ammonia nitrogen ($NH_4^+ - N$).

Ammonia nitrogen and organic nitrogen have common features; they are the most reduced forms of nitrogen and share the same oxidation state. A bacterial action (otherwise known as hydrolysis) involves nitrogenous organic compounds in degradation reactions.

In an aqueous solution, ammonia nitrogen can exist in two different types of compounds, i.e. as ammonium ions (NH_4^+), or free ammonia (NH_3). These compounds' molar concentration ratios differ based on a solution's pH and temperature. Free ammonia is assimilated and new cells are produced using heterotrophic and autotrophic biomass. Nonetheless, this biological process fails to achieve an acceptable level of ammonia removal in wastewater. Consequently, high nitrogen loads are usually removed using biological nitrification and/or denitrification.

Nitrification is the initial step in the biological removal of nitrogen. In nitrification, ammonia is oxidised to form nitrite, and after further oxidation, nitrate forms.

Figure 2.1 illustrates how organic nitrogen, which is present in raw wastewater, can be converted into ammonia, when proteinaceous matter undergoes bacterial decomposition and urea undergoes hydrolysis. Bacterial growth is present in all biological treatment systems. Since a low percentage of cell dry mass is comprised of nitrogen, assimilation of some ammonia nitrogen into the newly formed cells may occur. Cell autoxidation and lysis can also happen, depending on the procedures used in treatment, and the loading condition. Through lysis and autoxidation, a fraction of the ammonia utilised in cell synthesis returns to the liquid. Richard and Sedlakn (1991) state that removal of any residual assimilated nitrogen from the system can be achieved via the wasted biological sludge or net growth.

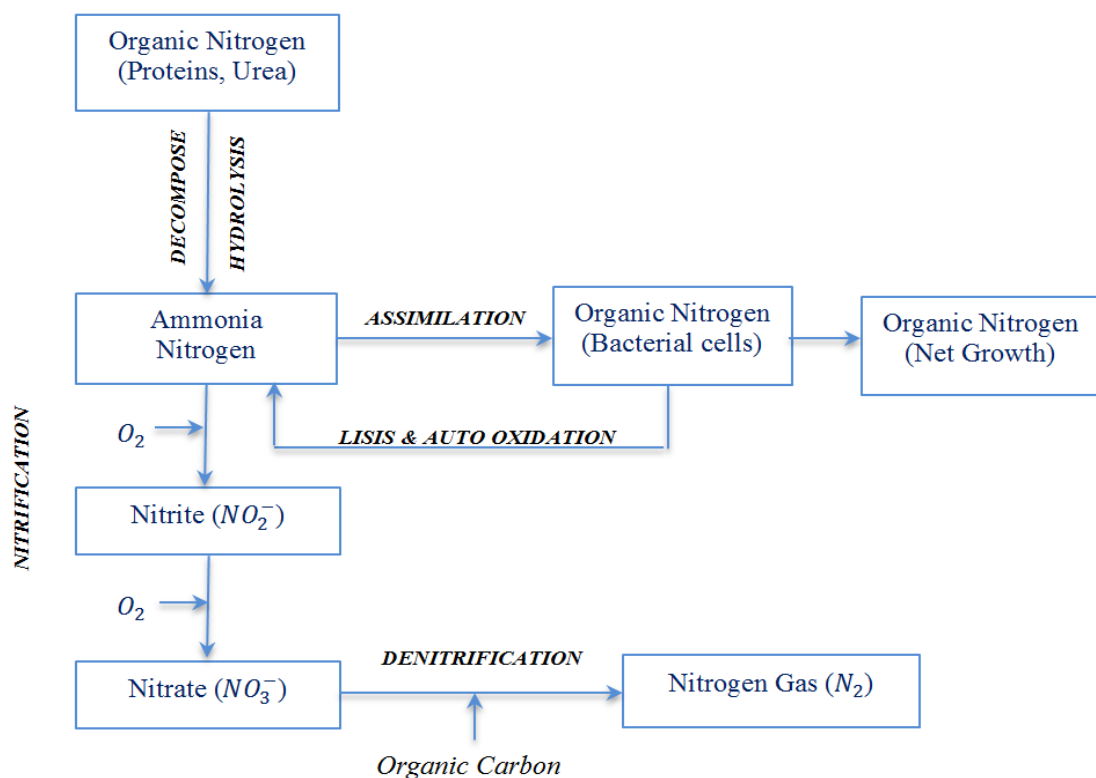


Figure 2.1: Nitrogen transformations (Sedlak, 1991)

In some specific conditions, oxidisation of ammonia nitrogen can produce nitrates in a two-step process. This process (nitrification), which usually requires oxygen, is performed by two groups of microorganisms (nitrifies). The resulting nitrates can then be converted into nitrogen gas, in a process referred to as denitrification. The conversion of nitrates into nitrogen gas is achieved by denitrifying microorganisms in the absence of oxygen. For this to occur, a source of organic carbon is a mandatory requisite for the denitrification process. Once produced, the nitrogen gas is released into the atmosphere. However, the effluent still has a small residue of non-degradable soluble organic nitrogen. In the nitrification stage, the impact of oxygen on the process of nitrogen removal should be taken into account; in particular, how it impinges on the rate of growth of the nitrifying bacteria. If the oxygen concentration is high, its permeation into the floc gets higher, thereby augmenting the rate of nitrification.

2.1.3 Biological phosphorous removal

The biological removal of phosphorous is usually conducted to control eutrophication, since phosphorous as a limiting nutrient in freshwater systems acts. Prior to 1980, the most common method for the chemical removal of phosphorous involved using alum or iron salts. However, the biological removal phosphorous was encouraged after the method proved successful in full-scale plant removal of phosphorous. Some of the core advantages of the biological removal of phosphorous include: it is cost efficient and results in the production of less sludge.

The strategy used in the removal of natural phosphorous is also used for the control-anoxic treatment of ammonia and nitrogen. *Bacterium acinetobacter* is the main organism used in this case. It is unclear whether an anoxic period stresses the bacterium,

or whether the anoxic period encourages it to use other sources of carbon to prepare for growth, and then retains the surplus phosphate to facilitate future growth. The removal of phosphorous and nitrogen in a wastewater treatment plant does not take place simultaneously. This is because nitrate interferes with the uptake of phosphorous, and as a result, phosphorous removal is only possible after nitrate removal. Additionally, true anaerobic conditions are required for the removal of phosphorous. An extra carbon source is needed to facilitate nitrate reduction and the uptake of phosphorous. As Russell (2006) explains, in the anaerobic process, bacteria initially release their own extracellular phosphorous and then uptake more phosphorous than they initially released.

Sedlak (1991) made the following observations regarding the biological removal of phosphorous:

- A myriad of bacteria wield the ability to store huge amounts of phosphorous in the form of polyphosphate.
- Fermentation products, such as volatile fatty acids (VFAs) can be assimilated, providing storage for phosphorous by PAOs in anaerobic conditions.
- Energy is generated when polyphosphate storage and storage products are oxidised in aerobic conditions.

Different types of phosphorous exist in wastewater in the form of phosphates. There are several criteria used in the categorisation of these types of phosphorous. In regard to their physical attributes, the types identified are disintegrated and particulate, and in regard to their chemical attributes, the types identified are dense phosphate, orthophosphate, and organic phosphate (Russell, 2006, Sedlak, 1991).

In the anaerobic phase, carbon is taken up by PAOs thereby leading to the production of PHAs which is then stored. So as to get the energy required for this process intracellular polyphosphates are degraded which leads to release of orthophosphate ($O\text{-}PO_4$). Some energy is also derived from the cell's glycogen (Figure 2.2).

In the aerobic phase, metabolism of the PHA which is stored and this provides energy needed for oxidation as well as carbon needed for the growth of new cells. This also leads to the production of some glycogen. The released energy is used in to remove soluble $O\text{-}PO_4$ from solution so that it can be incorporated into polyphosphates in the bacterial cell. Removal of phosphorous is facilitated by the formed biomass, which has high polyphosphate storage.

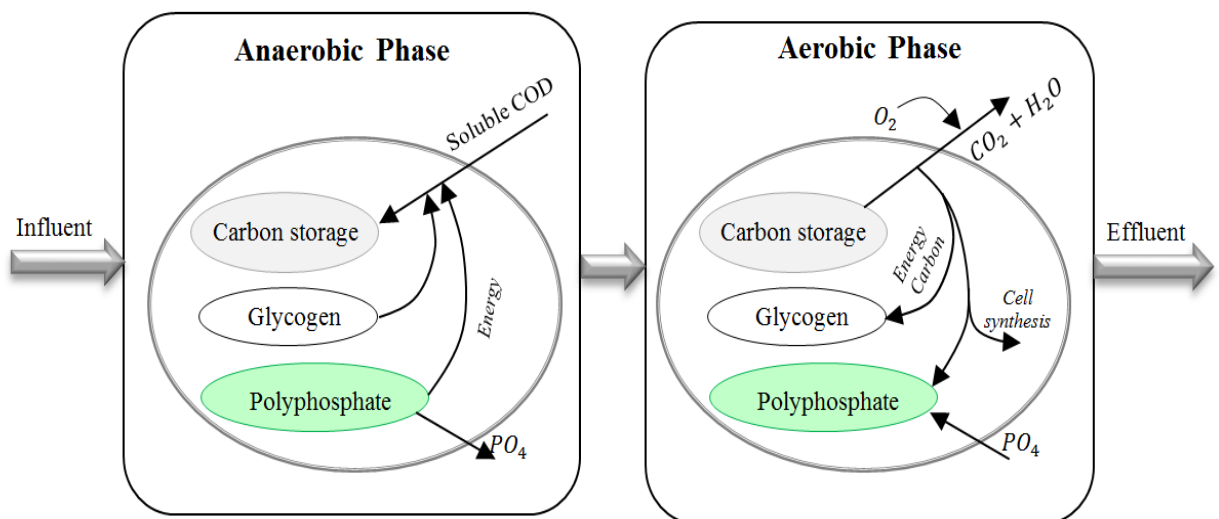


Figure 2.2: Principle of biological phosphorous removal. (Adapted from Chai, 2008).

Phosphorous forms part of the biomass composition of bacteria because it is needed in the DNA replication of bacteria. The removal of phosphorous in an activated sludge system is done using a particular group of heterotrophic bacteria referred to as polyphosphate accumulating organisms (PAO). The reason why they are used is because they wield the ability to store huge amounts of polyphosphate.

2.1.4 Biologically induced phosphate precipitation

The microbial reactions, which take place in wastewater treatment plants, lead to the precipitation of phosphate. In the activated sludge process, microbial activity in the aeration tank facilitates the precipitation and subsequent removal of phosphate from wastewater.

The precipitation of phosphate also takes place in denitrifying biofilms. As Arvin and Kristensen (1983) explain; this is because the denitrification process raises the level of alkalinity in a biofilm, leading to the precipitation of calcium phosphate.

The rate of precipitation, as explained in Arvin and Kristensen (1983) is directly proportional to the concentration of phosphorous in the system. Consequently, for the release of phosphorous in a polyphosphate pool to be high under anaerobic conditions, the phosphate concentration should be increased.

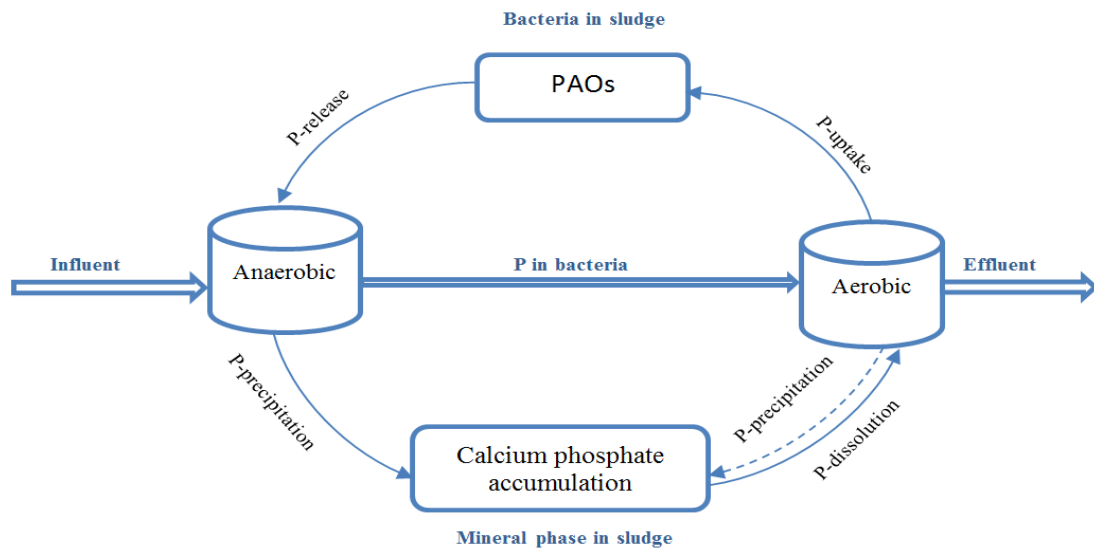


Figure 2.3: Phosphate accumulation by the EBPR process (Arvin, 1983)

To achieve the net removal of phosphorous, it is imperative to ensure that pH and calcium activity (among other factors) are maintained in a manner that prevents the re-dissolution of precipitated phosphorous under aerobic conditions. Figure 2.3 illustrates this mechanism.

EBPR's most noteworthy drawback pertains to the reversible nature of biological phosphate storage. Organisms break down internal phosphorous content, and then it can be re-released into the environment. The sludge should be handled with extreme caution. Reddy, (1998) stresses that it is imperative to limit the sludge retention times (SRT) in the settler, and to provide sufficient oxygen to the aerobic phase and the basin's outlet, to avert the occurrence of anaerobic conditions in the secondary clarifier (Baetens, 2001).

2.1.5 Sequencing batch reactor (SBR)

A sequencing batch reactor (SBR), described simply, is an activated sludge process that facilitates the stages that enable aeration and sludge settlement in one location. The variety of operating stages allows aerobic, anaerobic or anoxic conditions to exist, which specifically supports the propagation of desirable microorganisms.

There are three methods for achieving the removal of nitrate in the SBR process as well as other batch transfer processes. These include: (1) reducing nitrate by means of a mixed fill period that is non-aerated; (2) creating cycles of aeration where, aeration is intermittent during certain periods of reaction; and (3) lowering the concentration of DO during operations. The most effective method for removing nitrate is to enable denitrification during mixed fill periods that are not aerated. The bulking of filaments is also prevented with this method. Since the SBR tank's decant volume ranges between 20 and 30%, the majority of the nitrate generated in the earlier aerobic cycle stays in the

tank. Subsequent to decanting, McCarty and Smith (1986) assert that residual nitrate mass can be reduced in the fill period if the availability of time and BOD is sufficient. A second aeration time could enhance the removal of any remaining organics in the reactor (Jung et al., 2004).

SBRs are known, not only for ease of sludge manipulation, but also for properties such as the high removal rate of phosphorous and nitrogen from wastewater, and their considerable simplification of a treatment plant's technological arrangement. Wastewater is not aerated when the fill phase begins; and the basic parameters of the technological process, such as dissolved oxygen and the concentration of organic compounds, are a function of time (Janczukowicz et al., 2001). Moreover, to achieve successful removal of biological phosphorous and nitrogen, the length of the anaerobic period should be adjusted to achieve near-complete removal of easily biodegradable COD; and the length of the aerobic period should be sufficient for complete nitrification. Consequently, the total COD-loading rate must be kept high enough to attain a net growth of biomass in the reactor (Helness and Ødegaard, 2001). Figure 2.4 shows typical sequences with five common steps.

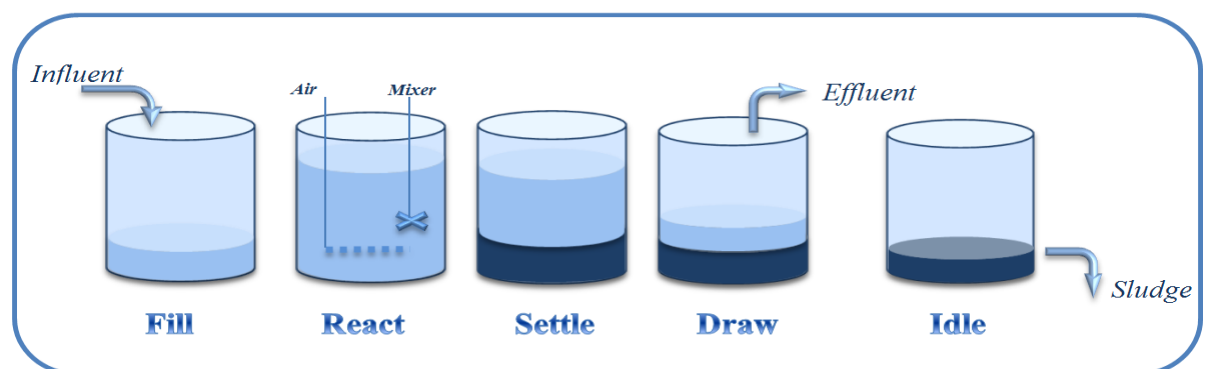


Figure 2.4: The order of events in the sequencing batch reactor (SBR)

- **Stage 1: Filling**

The cycle starts with the fill operation, which is the distribution of the influent wastewater throughout the tank, to provide a desirable reaction between the substrate and the microorganisms to trigger microbial activity as the wastewater enters the bioreactor. The duration of the fill can be selected according to a variety of conditions. If the time is short, the process will be analogous to a continuous flow system (successive tanks). As a consequence, organic materials and other components in the wastewater will lead to exposure of the biomass to high concentrations; however, these concentrations will decrease over time. By contrast, if the fill time is long, the system will behave in the same way as when completely mixing a continuous stream into the system. In this case, the biomass will be of low concentrations, comparable with other wastewater components.

- **Stage 2: Reaction**

With regard to the react stage, which comes after the fill is completed; this allows biomass and substrate consumption to act upon the wastewater components, as well the aeration. Compression or mixing can also be applied at this stage. It is desirable that the accomplishment of each phase is specified separately; because of the influence of each on the behaviour of the process. Moreover, the reaction (aeration and mixing) can be included in the fill phase.

- **Stage 3: Settling**

After the reaction period, a sedimentation stage follows, with the important condition of the termination of any aeration and mixing. This means that solid-liquid segregation takes place. In addition, biomass authorised to settle and clear the effluent will appear

above the sludge. For this reason, there are no liquids entering and leaving the tank, and the sedimentation in a discontinuous system could be carried out more efficiently than in a continuous-flow.

- **Stage 4: Decanting (Draw)**

When sufficient settling has occurred, the elimination of treated effluent from a finite distance above the sedimentation of the sludge takes place to ensure the withdrawal. The amount of liquid and biomass reserved in the bioreactor comprises the biomass recycle for the next cycle. If a large volume is retained, relative to the influent volume (in order to provide nitrate for an initial denitrification period), then that volume is analogous to biomass recycle in a continuous process.

- **Stage 5: Idling**

Finally, an idle period is generally allowed in each cycle to provide flexibility. This final stage can only be used to pump the waste sludge, to reduce the volume, according to the time required to complete the cycle. The opening of the new fill terminates the idle phase, and begins a new cycle. Typically, the frequency range of waste sludge should be once every (60 -100 days) depending upon system design. The amount of liquid and biomass reserved in the bioreactor comprises the biomass reprocess for the next cycle. Chen et al. (2013) compared two dissimilar SBRs reactors in terms of their phosphorous removal performance, and found the enhancement of poly-P takes place when there is an increased energy requirement for bacterial preservation, due to an increase in idle time.

The system of a sequencing batch reactor for biological phosphorous removal is built by the creation of a sequence of anaerobic conditions, followed by aerobic conditions. This enables the system to perform the phosphorous removal without the need for any chemical additives. The system could be modified, as illustrated in Figure 1.2, to result in the combined oxidation of carbon and nitrogen. This modification would involve the introduction of an anoxic phase after the aerobic reaction phase.

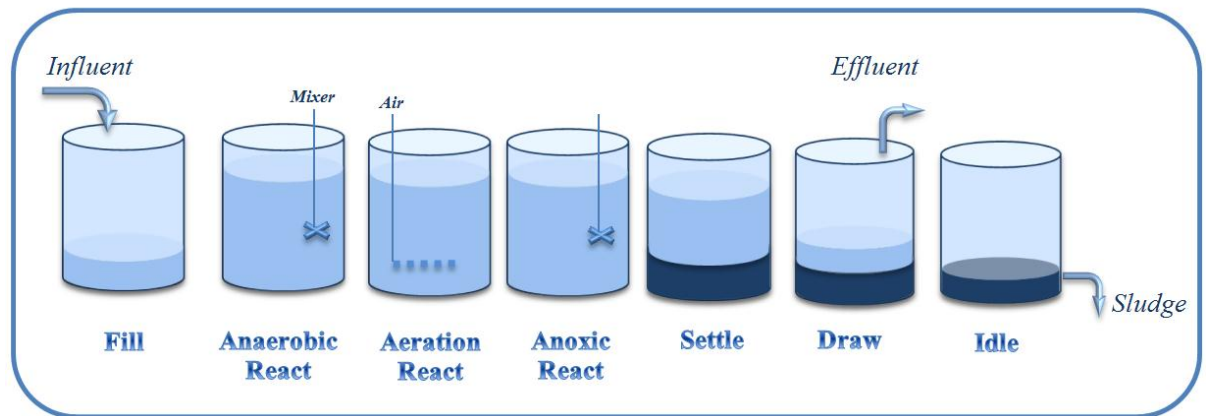


Figure 2.5: SBR for the removal of nitrogen and phosphorous

2.2 WWTP operation and control

2.2.1 Biological Growth Kinetics

A proper understanding of underlying biological growth kinetics is essential when designing and operating suspended and attached growth biological treatment processes.

As illustrated in Figure 2.6, there are four conceivable phases of the biological growth cycle. To become well acquainted with these phases, it is useful to consider a bacterial population in a closed bottle with a fixed amount of food. In the beginning (lag phase) the bacteria will take some time to become accustomed to their environment prior to the initiation of their reproduction. In the log growth phase, there is ample food (substrate), leading to an exponential reproduction of cells. In the stationary growth phase, food gradually becomes limited, and the rate of growth becomes equal to the rate of death. In the log death phase, food becomes scarce and the bacteria start to consume each other for food (this is referred to as endogenous growth). A biological wastewater treatment process is comprised of different generations of bacterial populations in competition with each other at different phases (Templeton and Butler, 2011).

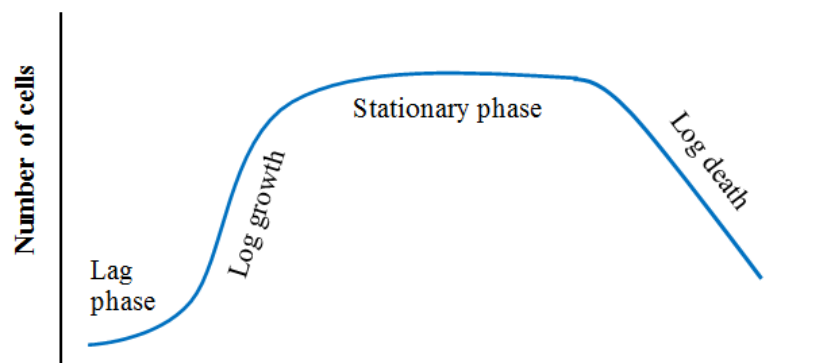


Figure 2.6: The biological growth cycle

2.2.2 Effect of Sludge Retention Time (SRT)

A higher amount of SRT is needed in nitrification than in carbonaceous oxidation, especially if the temperature of the wastewater is low, as this would decelerate the nitrifiers' growth rate. When the nitrifiers' growth rate is slow, a higher SBR is required to assist the nitrification process. To change the SRT the measure of sludge wasted every day should be controlled, and effluent suspended solids (ESS) lost accounted for.

According to McCarty and Smith (1986), the SRT factor increases the flexibility of operational variations, and enables the augmentation of nitrifying bacteria, which is necessary when dealing with peak loadings.

Sedlak and Richard, (1991) state that during the denitrification process, the majority of bio-degradable organics are consumed. As a result, the denitrification process' most significant benefit is satisfaction with the allocation of the oxygen demand for carbonaceous matter.

To achieve an ever better control of SRT, it is imperative to calculate the mixed liquor suspended solids (MLSS) and change in the quantity of sludge wasted.

$$SRT = \frac{\text{Sludge in Reactor } (gVSS)}{\text{Sludge waste } (\frac{g}{day})} = \frac{V_0 X}{(Q_W X + Q_E X_E)} \quad 2.5$$

Where:

V_0 is the volume of each SBR (l).

X is the mixed liquor suspended solid (MLSS) concentration at end of one cycle (mg/l).

Q_W is the amount of sludge wasted per day from SBR (l/day).

Q_E is the amount of discharged effluent per day from each reactor (l/day).

X_E is the effluent suspended solids concentration in treated effluent (mg/l).

2.2.3 Effect of Temperature pH extension

Similar to most biochemical reactions, temperature is one of the factors that impinges on nitrification kinetics. The most distinct impact of temperature is usually seen in the maximum specific growth rate $\mu_{m,A}$. Based on experiments, a conclusion has been reached that states an Arrhenius type equation in the range of 7-30°C can model the impact of temperature on $\mu_{m,A}$.

$$\mu_{m,A}(T) = \mu_{m,A}(20^{\circ}\text{C})\theta^{(T-20^{\circ}\text{C})} \quad 2.6$$

T represents the actual temperature, and $\mu_{m,A}(T)$ represents the maximum specific growth rate of autotrophic biomass at T, while θ represents the temperature coefficient. The literature has provided several values ranging from 1.08 to 1.23 for θ (Orhon, 1997).

The ASM2d and Biological Nutrient Removal Model No. 1 (BNRM1) were employed to understand the impact of pH on enhanced biological phosphorous removal in an anaerobic/aerobic SBR laboratory (Serralta et al., 2004, Serralta et al., 2006). The findings showed that an increase in the amount of phosphorous increased the pH level. To accurately forecast the transformation of phosphorous in SBR, the ASM2d model should include a pH impedance step as well.

To effectively tackle degeneration and upgradation, an important sector of the activated sludge model must be used. In lysis reactions, the bacteria are recycled for used as substrates of elements in the ASM2 model (Van Veldhuizen et al., 1999).

Serralta (2004) further developed ASM2d to include a chemical model with the ability to calculate the pH value of biological processes. This development took account of all the components that impinge on the pH value, as well as an ion-balance to facilitate the calculation of pH value and disassociation of species. The new version of ASM2d took into account the stripping of carbon dioxide, where the calculation of the carbon dioxide's mass transfer coefficient was based on the coefficient of oxygen at the aerobic stage. The actions of glycogen under aerobic conditions were also taken into account in the new version; glycogen was not considered in ASM2d despite recognition of its significance as a carbon storage material for PAO (Serralta et al., 2004).

2.2.4 Sludge Wasting in SBRs

Sludge wasting is important step in the SBR operation, and one that greatly affects performance. Wasting is not included as one of the five basic process steps, because there is no set period within the cycle dedicated to wasting. The amount and frequency of sludge wasting is determined by performance requirements, similar to a conventional continuous-flow system. In an SBR operation, sludge wasting usually occurs during the react phase, so that a uniform discharge of solids (including fine material and large floc particles) occurs. A unique feature of the SBR system is that it removes the need for a return activated-sludge (RAS) system.

One hour or less is required to remove any BOD dissolved, because of the batch kinetics of domestic wastewater treatment. This usually leads to a moderately low early concentration of dissolved BOD. According to WEF (1998), the time required for SBR aerobic reactions in nitrification range between 1.0 and 3.0 hours. There is no similarity

between SRTs, SBR and the process of continuous-flow activated-sludge. Similar to SRT, the efficiency of SBR is expected to be higher, because of its batch kinetics. However, biomass is not exposed to aeration for longer periods, thus lowering the effectiveness of the SRT.

The utilisation substrates, as well as the rate of oxygen demand reduce with time; this is because the concentration of the substrate changes as time progresses. According to Henze (2008), the design of the aeration system is supposed to reflect the changing rates of oxygen demand.

2.2.5 Effects of SBR Cycles

When the influent is supplied to a reactor tank, the amount of ammonium would theoretically be converted into nitrate at the end of aerobic stage. This conversion would work under the classic anaerobic–aerobic condition of the SBR. In addition, to reduce the nitrate level in SBR reactors to zero, the process requires the addition of an external organic carbon, such as acetate, to the input phases, after the aerobic stage contributes to an extra anoxic stage for denitrification before effluent discharge. However, this consideration could lead to an increase in operational rate, due to the use of chemicals. It is noted that N removal can be more effectively carried out by denitrification during the anoxic stage than at another stage, but this does not mean that the N removal in anaerobic–aerobic reaction should be assumed negligible.

Figure 2.7 shows that exposure of mixed liquor in the anaerobic/aerobic sequence, leads to the accumulation of high levels of phosphorous within cells, as well as other micro-organisms able to absorb and store phosphorous in the aerobic zone. This storage is then

used in the anaerobic zone, to produce the energy needed for the fermentation process. On the other hand, a fraction of soluble BOD is transformed to simple organic components through the anaerobic zone. As a result, there is decreased BOD in the anaerobic sequence, even if the electron acceptors are not present.

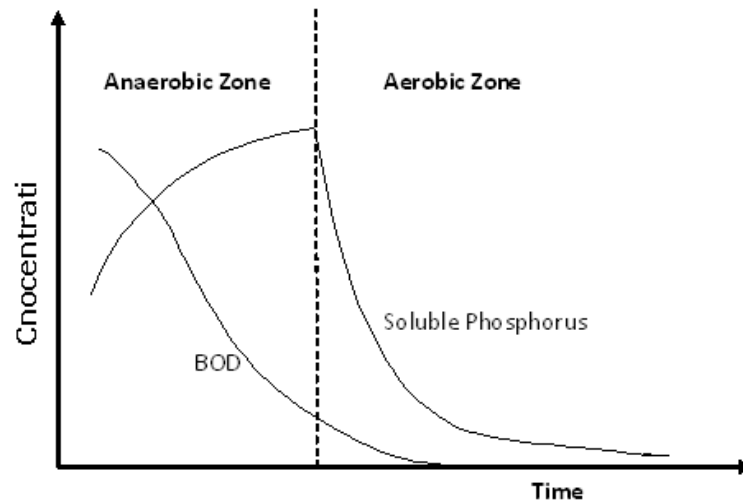


Figure 2.7: Variation of soluble BOD and phosphorous concentration

The secondary wastewater feed into the SBR system at the beginning of anoxic phase, and the complementary nature of carbon and low redox potential in the new feed, would further strengthen the denitrification intensity; thus, converting most of the nitrate oxidised in the first aerobic stage into gaseous nitrogen. As a result, with two feeding inputs, the capability for nutrient removal would be increased to guarantee low nitrate levels in the final effluent.

As might be anticipated, and as Figure 2.8 illustrates, during the fill stage (where wastewater is going to be added to the volume remaining from the previous cycle), the concentrations of soluble organics (COD) and ammonia- N rise rapidly due to distributed wastewater inflow. On the other hand, the concentration of nitrate-N that comes from the volume retained from the previous cycle drops, as it provides electron

acceptors for the biodegradation of the readily biodegradable substrate. It should be noted that the complete oxidation of carbon during the fill period, and the reaction rate, is relatively high enough to limit the accumulation of soluble organics.

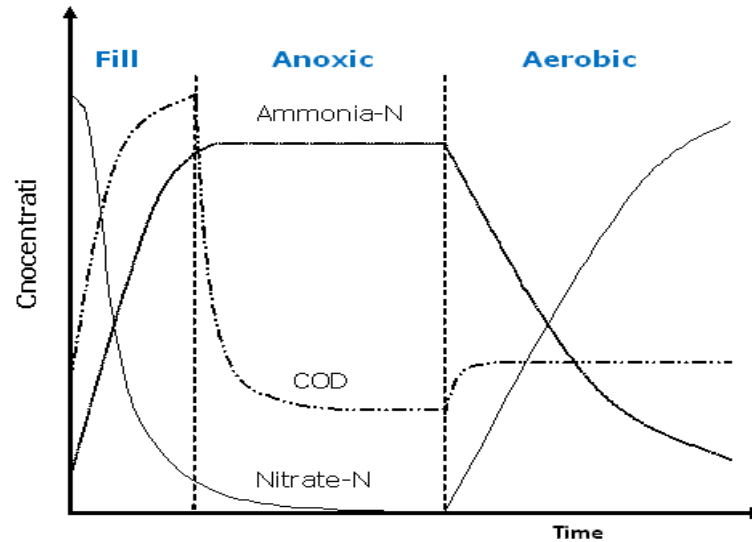


Figure 2.8: Ammonia, Nitrate and COD concentration behaviour during SBR phases.

In terms of the anoxic and aerobic zone; during the anoxic stage, alternative carbon sources are needed, the mass of nitrate-N retained from the previous cycle will attain a balance with the mass of the readily biodegradable COD which has been added. As a result, the soluble organics and nitrate-N will deplete rapidly, then a small amount of soluble organic matter will remain, while all the nitrate-N will be removed.

During the aerobic phase, nitrification is considered to be the main occurrence affecting the aerobic reaction. The soluble organics change slightly because of their production in hydrolysis reactions. This fact depends on whether the aerobic stage come after an anoxic or anaerobic phase. Moreover, there is an increase in the rate of ammonia-N, while the rate of nitrate-N decreases; however, the reaction behaviours are almost linear.

2.3 Model of wastewater treatment process

2.3.1 Modelling Nitrogen Removal

Seven components need to be considered to deliver a simple example of the biological removal of carbon and nitrogen from wastewater. These are: a heterotrophic biomass, soluble carbon, water, and oxygen as well as an autotrophic biomass, nitrate (NO) and ammonia (NH).

As illustrated in Figure 2.9, there are two sequential steps for the removal of nitrogen. The aerobic growth of autotrophs leads to the consumption of soluble carbon, ammonia, and the dissolution of oxygen, which leads to the production of additional nitrates and biomass in solution. At times, this first step is further subdivided into two, where nitrites are produced in the first sub-step and nitrites are oxidised into nitrates in the second sub-step. In the second major step, anoxic heterotrophs use nitrates as sources of oxygen, to grow and produce, which leads to the production of additional nitrogen gas and biomass (Olsson and Newell, 1999b).

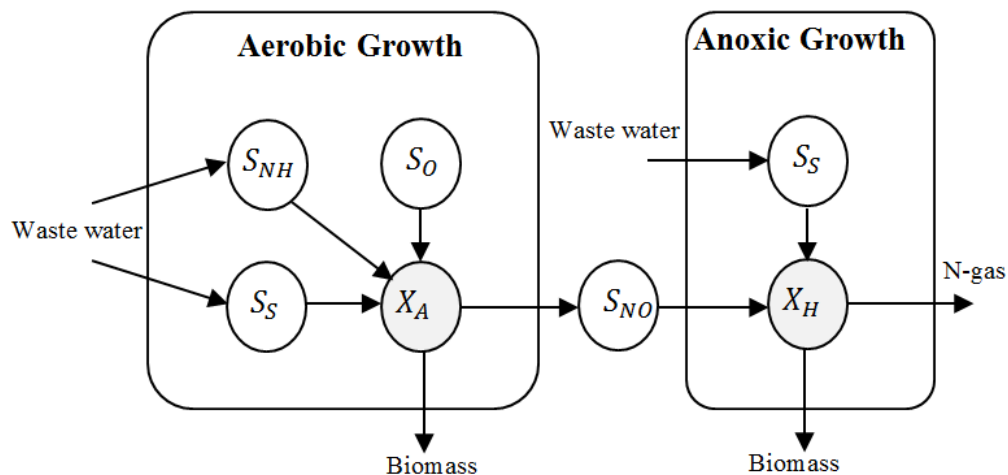


Figure 2.9: Nitrogen removal

2.3.2 Modelling Phosphorous Removal

As illustrated in Figure 2.10, the intricacy of the process of removing phosphorous is much greater, and a diagrammatic representation is necessary to explain it.

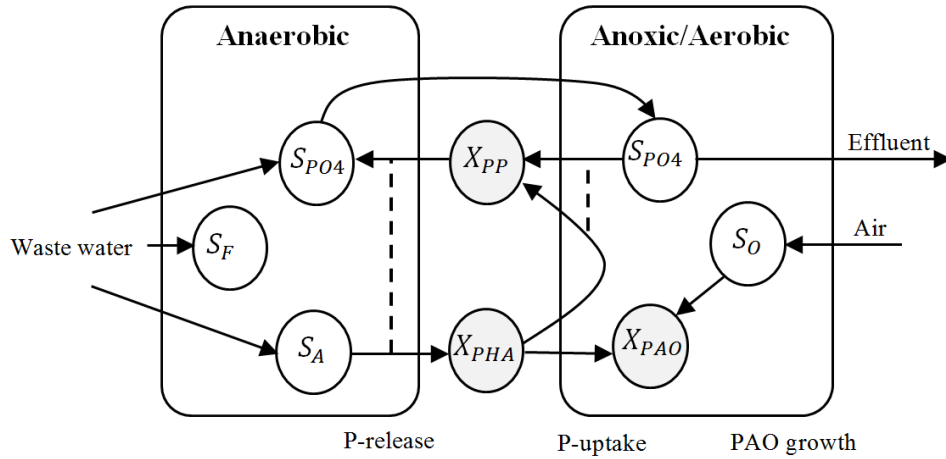


Figure 2.10: Phosphorous removal

In Figure 2.10, there are X components, all of which are elements of the phosphorous accumulating organisms (PAOs). The two dashed lines represent transformational links.

There are four basic mechanisms illustrated in the figure (Olsson and Newell, 1999b):

- COD that is fermentable, S_F , ferments to produce volatile fatty acids (VFA), S_A , which can be used for the storage of carbon as polyhydroxyl-alkanoates (PHA), X_{PHA} by PAO microorganisms.
- There is simultaneous release of phosphorous from polyphosphate (PP), X_{PP} , and conversion of VFA into PH.
- PHA and dissolved oxygen enable the uptake of phosphorous from a solution to form PP, S_{PO_4} .
- PHA and dissolved oxygen also enable the growth of PAO biomass, X_{PAO} .

One of factors that complicate the process is that there is competition for the VFA by heterotrophs and the denitrification process. It is imperative to maintain the conditions that facilitate the growth of PAO as well as the higher uptake than the release of P, so as to acquire an efficient removal of P. The maintenance of these conditions is not entirely scientific, because the correct conditions remain the subject of debate and may also be contingent on the wastewater itself, as well as other environmental factors, such as alkalinity, temperature and redox potential.

In comparison with the removal model for carbon and nitrogen, there were five more mass balances and states produced in the P removal model process (i.e. S_A , PP , S_{PO_4} , X_{PAO} , and X_{PHA}).

2.3.3 Modelling Prefermentation

Fermentation (otherwise known as acidogenesis) is a process that entails degradation of sugars, amino acids, and some fatty acids. Organic substrates take on the role of electron donors and acceptors. Fermentation leads to the generation of products such as propionate, hydrogen, carbon dioxide, and acetate. These can undergo further fermentation, leading to the generation of hydrogen, carbon dioxide, and acetate. The products generated after fermentation (hydrogen, carbon dioxide, and acetate) are used in methanogenesis (the formation of methane). McCarty and Smith (1986) assert that when propionate undergoes further fermentation to generate hydrogen, carbon dioxide, and acetate, free energy is used up, and this requires low concentrations of hydrogen, otherwise the reaction will not continue (Riffat, 2012).

Figure 2.11 shows IAWQ Activated Sludge Model No 2 model, which gives a simple explanation of fermentation as two sequential reactions (Olsson and Newell, 1999b).

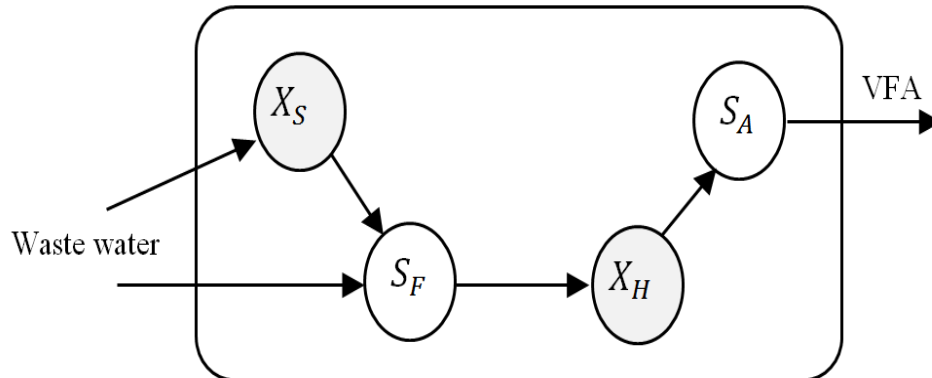


Figure 2.11: Fermentation model

Moreover, fermentation refers to the process by which organic carbon breaks down anaerobically into VFA, thus promoting the uptake of biological phosphorous. The process can also entail two other mechanisms. When the organic carbon being used is insoluble (which is usually the case), it must first be hydrolysed to make it soluble. The breaking down of VFA into methane is another less desirable mechanism. Acidogens, which are responsible for the production of VFA, and methanogens, which are responsible for the breaking down of VFA are the two types of organisms used. These organisms are also used indirectly for the secretion of enzymes required in hydrolysis reaction.

The first step involves enzyme catalysed extracellular reactions that hydrolyse insoluble organic carbon, X_S , to form a soluble fermentable substrate, S_F . In certain cases, this step may not allow for mass transfer. An example of such as case is that, if the solid particles are large, they then have a small surface area. In the second step, i.e. fermentation, fermentable organic carbon is converted into volatile (short chain) fatty acids, S_A , using heterotrophic organisms.

2.4 Process optimisation

2.4.1 Orthogonal collocation method

The orthogonal collocation method is depended upon to meet the objective of transforming partial differential equations into a group of algebraic equations that can be solved using an external nonlinear solver. This collocation method estimates solutions to differential equations' through the linear integration of basic functions, which are established by requiring that the ODE satisfy a discrete set of mesh points. Satisfaction of boundary conditions is also required.

Finlayson (1980) was responsible for the simplification of mathematical principles used to develop numerical solutions to assist the activated sludge process (Finlayson et al., 2000). This technique was proven to be more superior in terms of time taken to compute, and the accuracy of the solution when compared with other weighted residual methods. There have been numerous successful applications of this technique during the development of numerical solutions for dynamic models of industrial chemical processes.

Heinemann (1974) presented two ways in which orthogonal collocation method applications for chemical reaction engineering can be viewed. The first way entailed refining successive calculations using additional collocation points to calculate a numerical method, upon which convergence to the exact answer can be viewed as estimation. The second way considers the first approximation, and makes it analytical, thus affording valuable insight regarding the solution's qualitative behaviour. Therefore, the numerical method is used in the acquisition of approximate solutions.

2.4.2 Genetic algorithms

According to Godfrey (2004), John Holland developed the first genetic algorithm (GA) technique in 1965. GA methods of search and optimisation operate by imitating the chromosomal processing and evolutionary principles in natural genetics. The search for a GA begins with a random group of solutions that use a binary string structure for coding. The solution is allocated fitness in direct correlation with the objective function of the problem. Using three natural genetics operators of (i.e. crossover, reproduction, and mutation), a new population of solutions can be formed. The GA conducts successive application of the three operators in each generation, until fulfilment of a criterion for termination. According to the global perspective, simplicity, and the inbuilt parallel processing ability of GAs, the application to manage numerous engineering problems has been quite successful in the last few decades.

The GA involves the use of a population of individuals to explore various regions of a solution space. Initially, the formation of a population is carried out randomly with the evaluation of the fitness of all every individual conducted through a fitness function. After the fitness evaluation is completed, selected individuals are subjected to genetic operations, such as crossover and mutation, depending on their respective fitness to produce the next generation of individuals to be subjected to a fitness evaluation. The process would be repeated continuously up to a point where an optimal solution is established (Wang and Wan, 2009).

2.4.3 Genetic algorithm approach

Traditional methods of search and optimisation result in a myriad of difficulties when engineering problems arise. The major difficulty arises when one algorithm is applied to solve a number of different complex problems. The design of a traditional method only enables them to solve a specific category of problem efficiently.

Although similar general algorithmic procedures are used in the development of GA systems, the design and implementation of each GA system differs somewhat, as it uses a variety of compilers and number generators at random. As a result, the optimisation of a model by two systems cannot be exactly similar. Significant differences also impinge on the solution process, such as the parameter options that are espoused in each solver. The most important parameters include: the method of selection, the rate of crossover, the rate of mutation, the scheme of recombination, and the population size.

2.4.4 Typical characteristics of genetic algorithms

- The operational procedure of a GA is based on the variable groups' codes (artificial genetic strings), instead of the variables themselves.
- Its operational procedure is based on a group of potential solutions (population), rather than attempting to enhance one single solution.
- It does not base its operational procedures on information that has been acquired directly from the object function, the derivatives of the object function, or any other secondary information (Olsson and Newell, 1999a).
- Instead of using deterministic rules it uses probabilistic transition rules (Rangel-Merino et al., 2005).

2.4.5 Genetic Algorithm Operators

GAs, as in figure 2.12, can furnish satisfactory results for practical problems, based on three operators, which include Reproduction (selection), Crossover and Mutation.

Reproduction: the goal of this process goal is to make sure that the genetic information, which is kept in artificial fitness strings, continues to exist until the next generation. Typically, population's string is given a value in accordance with its ability with regard to the object function. This value can be selected later, as the parent, if a new generation is needed. Although supplementary information (derivatives) about the function undergoing optimisation is not required in GAs, it is essential to be well acquainted with the existing global optimal.

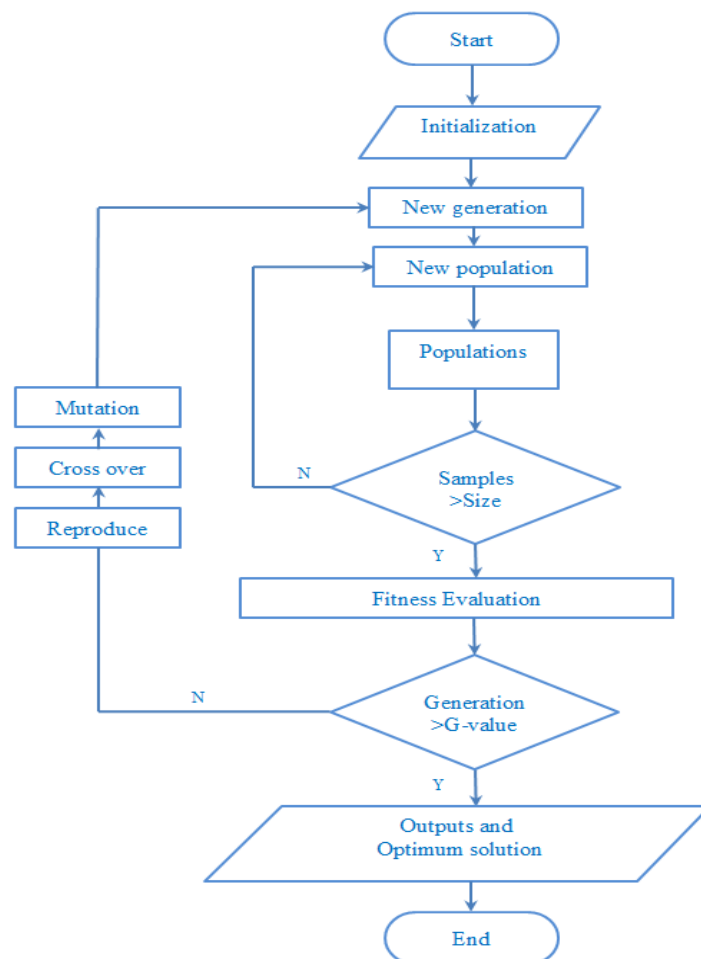


Figure 2.12: Flow chart of genetic algorithm process

Crossover: GAs typically include numerous individuals, which in most cases range from dozens or hundreds. Similar to biological populations, mating between two individuals can occur. To mate, each individual is made to “crossover”, and this produces offspring with similar genetic information. A random number is selected when finding a crossover point. If the random number 2 is selected as the crossover point, the alleles of two individuals are swapped among themselves subsequent to the second bit position in every chromosome, as illustrated below:

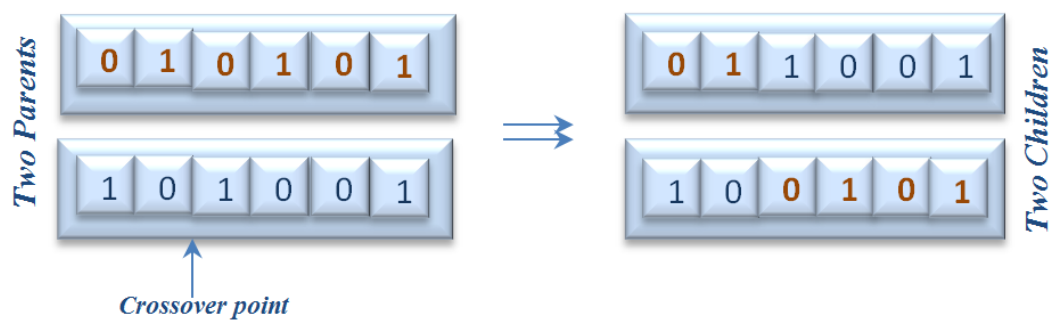


Figure 2.13: Figure Illustration of crossover in a binary GA.

Mating (i.e. crossing over) occurs between the two parents, leading to the creation of two children. The genetic information of both parents is transferred to each child. This leads to the death of the parents, leaving the children to continue the process of evolution. This process is referred to as the creation of a new generation, in a GA. The fitness of the children will vary, just as with biological processes. The likelihood of death for children with low fitness is higher than for those with high fitness. Children with high fitness survive, then mate (cross over) with other high-fitness children, which leads to the formation of a new generation. This process repeats, until the GA has established a satisfactory solution.

Mutation: In biology, mutation is relatively uncommon; at least to the extent that it noticeably impinges on offspring. Mutation is also quite uncommon when implementing GAs (about 2%). It is, however, impossible to state a correct setting for the rate of mutation in GAs. The rate of mutation is contingent on factors such as encoding, the problem, the size of the population, and others. Mutation, irrespective of its frequency, is significant, as it allows the exploration of potential solutions through the process of evolution. If a population lacks some genetic information, it might be possible to inject that missing information through mutation. Mutation is of paramount importance in biological evolution, and also in GAs. This is because the population sizes are so small, causing inbreeding to become problematic; thereby, resulting in dead-ends in the evolutionary process. The size of a population in biological evolution can be in the millions, while in GAs the population only exists in the dozens or hundreds.

According to Simon (2013), the implementation of mutation begins with the selection of a probability for mutation, perhaps 1%. The meaning of this is that each bit of the offspring produced in the crossover has a 1% chance of turning into the opposite value (0 turns into 1, 1 turns into 0). One of the attributes of mutation is its simplicity. However, the selection of a practical mutation probability is of utmost importance. If the mutation probability is set too high, the GA starts to resemble a random search, thereby compromising the efficiency of any solution to the problem. On the other hand, if the mutation probability is set too low, complications pertaining to inbreeding and dead ends in the evolutionary process arise, and this also compromises the efficiency of any solution to the problem.

2.5 Literature review of state-of-the-art of ASM modelling

The purpose of this literature review is to provide an overview of the relevant research studies by others associated with the various biological processes of wastewater treatment, which will be addressed later in this study.

The benefits of implementing the activated sludge model were confirmed by the International Association on Water Pollution Research and Control (IAWPRC), formerly known as IAWQ. The Mathematical Modelling for Design and Operation of Biological Wastewater Treatment task group was established in 1983, by the IAWPRC, with the intention of encouraging extensive use of the model among practitioners. The responsibilities assigned to this task group included:

- Reviewing literature to identify extant models.
- Establishing a consensus on matters pertaining to the easiest and most appropriate approach to modelling.
- Establishing a low intricacy mechanistic model capable of designing and operating activated sludge systems to be used for denitrification, nitrification and carbon oxidation (Makinia, 2010).

2.5.1 Standard Model for Activated Sludge Processes

From the mid-1980s onwards, the EBPR process started to gain popularity as numerous insights emerged. As a result, an new version of the activated sludge model, which took into account the removal of biological phosphorous, was established in 1994 (ASM2) by Henze et al. (1995). It also included a simple model for the removal of chemical phosphorous. Henze et al. (1999) re-modified ASM2 to form ASM2d, and later, ASM3

(Gujer et al., 1999, Henze et al., 2000). ASM3 incorporates additional advanced knowledge regarding internal storage of compounds that play a key role in an organisms' metabolism. However, ASM3 does not have the ability to remove biological phosphorous. Details regarding ASM2 and ASM2d are provided in the following section, and it should be noted that new versions of the model are in development.

- ASM1

Activated Sludge Model No. 1 (ASM1) was specifically designed for municipal activated sludge WWTPs to explain how organic carbon compounds and N are removed, with simultaneous nitrate and oxygen consumption working as electron acceptors. ASM1 aims to describe sludge production adequately and efficiently. It measures concentrations of organic matter using chemical oxygen demand (COD), and then divides the huge assortment of organic carbon and nitrogenous compounds into a limited number of fractions, based on their biodegradability and solubility. Regardless of the extensive research into biological phosphorous removal prior to the development and final release of ASM1 in 1987, its theoretical status was not sufficient for inclusion in a standard model.

Dold and Marais (1986) meticulously evaluated this model, and proposed structural modifications made to it, particularly regarding how the fate of organic nitrogen was modelled.

In the last ten years, a number of deficiencies associated with the ASM1 model have been identified through its extensive implementation in research and practice. A new model, referred to as the ASM3 was established by the International Association on

Water Quality (IAWQ) task group to rectify the deficiencies identified (Gujer et al., 1999) .

In the formulation of the final form of ASM1, the proposed modification suggestions were considered (Henze et al., 1987). Regardless of the comparable complexities concerning their ability to simulate biological processes (i.e. denitrification, nitrification and carbon oxidation), ASM1 and ASM3 manifest conceptual differences. The most noteworthy difference is that unlike ASM1, ASM3 does not consider heterotrophic growth on external substrate directly. Makinia's (2010) appraisal claims that both models have a limitation, in that they do not take account of the Enhanced Biological Phosphorous Removal EBPR process.

Eight years after the establishment of the ASM1, an extended version, referred to as ASM2 or EBPR, was established by a similar IAWQ task group (Henze et al., 1995a). When evaluating the difficulties and developments experienced when modelling the EBPR processes, Ekama and Wentzel (1999a) referenced ASM2, concluding that recent developments in this area did not support a significant improvement in the predictive aptitude of ASM2. Henze et al. (2000) state that the ambiguity of the role of denitrification regarding the EBPR process persisted after the completion of the ASM2, and as a result, a decision was made not to include the element.

- **UCTPHO model**

The ASM1 and UCTOLD model were combined to form The University of Cape Town model UCTPHO (Wentzel et al., 1992), to accomplish the biological removal of excess phosphorous. This phosphorous removal process was included, to interpret microscopic reactions in biological nutrient removal activated sludge. The principles of this

prototype have been employed to understand and forecast PAO processes and create an internal Polyphosphates (poly-P) store. According to Wentzel et al., 1992, UCTPHO is a complex general kinetic model, used for nitrification and de-nitrification and biological removal of excess phosphorous (NDBEPR) processes. The model does not encourage the generation of PAOs with anoxic P uptake (Hu et al., 2003).

- ASM2

This system was a derivation of the ASM1 (Henze et al., 1987) and the UCTPHO models (Wentzel et al., 1992). ASM2 comprises 19 processes and 19 components. This level of intricacy was requisite to describe the multiple process configurations used for EBPR. Aiming to explain the behaviour of phosphorous, nitrogen, and organic matter in the SBR activated sludge process; Furumai et al. (1999) drew references from ASM2 and established an integrated dynamic mathematical model. This mathematical model supported the establishment of ASM2d, which is a revised version of ASM2 (Henze et al., 1999). The development of ASM2d was based on ASM2 (Henze et al., 1999, Gujer et al., 1995) and ASM1 (Henze et al., 1995a).

According to Chuang (1999), the activated sludge model ASM2 relies on the following approximations:

- The dispersed activated sludge comprised of X_H and X_{PAO} , whereas X_{AUT} acts as a biofilm sludge.
- The development of X_H and X_{PAO} illustrates an organisms development in this process, whereas X_{AUT} is not considered.
- The development of X_{PAO} only occurs at the aerobic stage using a PHA store. Additionally, nitrogen removal properties are not present in X_{PAO} .
- Phosphorous is transformed to Polyphosphate and then removed.

There is an observable increase in the generation and degeneration reactions of PAOs. If the main amount of phosphorous is non-existent, UCTPHO cannot be used to forecast the generation and biological phosphorous removal under phosphorous constrained conditions (Hu et al., 2003). The ASM2 removes this constraint through the addition of poly-P grouping reactions. In ASM2, the dispersion of bacteria is approximated. One of the most significant approximations concerns the tabulation of biomass. In the model currently in use, organisms that uses organic carbon are divided into two parts. These are X_H (heterotrophs) and X_{PAO} (phosphate-accumulating organisms).

A X_{AUT} label is placed upon the organism to make a complex substance from a simple one. According to the prototype, X_H can be formulated in both oxygen requiring and oxygen depleting steps, whereas X_{PAO} can only develop on a saved PHA with the help of oxygen. Therefore, heterotrophic biomass production is represented by the nitrate degeneration and oxidation of X_H and PHA oxidation of X_{PAO} . To date, there is almost no research on the organism dispersion of numerous bacteria (Wentzel and Ekama, 1997).

- Activated Sludge Model no. 2d (ASM2d)

According to Henze et al. (1999), this model is an improved form of the above model, and is used principally to explain the biological elimination of excess phosphorous, and nitrogen removal. The links between nitrates and phosphorous in the absence of oxygen are components of this model. Henze's et al. (1999) ASM2d is a re-modification of ASM2, that involves adding PAOs' denitrifying activity to improve the description of phosphate and nitrate dynamics. PHA is utilised for anoxic poly-P formation and anoxic PAO growth processes. The ASM2 for the growth of PAOs, and poly-P formation in the

presence of oxygen, was used in the formulation of these processes. In the absence of oxygen as a terminal electron acceptor, PAOs utilise NO_3^- 's reaction with phosphorous.

Stored polyphosphate (poly-P) acts as an energy source to improve PAOs' ability to rapidly uptake degradable substrates, and synthesise poly-hydroxyalkanoates (PHAs). Stored PHAs, as explained by Peng (2011), can then be used to facilitate excess uptake of phosphorous, and the growth of microorganisms in the aerobic zone.

- **Barker and Dold Prototype**

Barker and Dold (1997) put forward a standard model to eliminate the nutrients from the activated sludge. This model uses carbon-containing energy, nitrification and denitrification reactions based on the ASM1. Barker and Dold explained the biological phosphorous removal process using data previously collated by Wentzel et al. (1989). In addition, fermentation reactions readily change biodegradable chemical oxygen demand (RBCOD) to volatile fatty acids (VFAs). The Barker and Dold (1997) model was created to illustrate the workings of autotrophic nitrifying organisms (ANOs), ordinary heterotrophic organisms (OHOs), and PAOs. All the nitrification, denitrifications, biological excess phosphorous removal processes (NDBEPR) are significant here (Barker and Dold, 1997). The ASM2 and these phosphorous removal reactions are the same but some of their characteristics vary.

- **ASM3 with Bio-P Module**

To model the phosphorous removal process biologically, the Bio-P unit was added to ASM3 (Rieger et al., 2001). The ASM2d model assumption is used to formulate the biological phosphorous removal process in ASM3. ASM3 combined with the Bio-P module uses hydrolysis, autotrophic and heterotrophic reactions as in the ASM3 model.

Although S_S is not fermented by heterotrophic organisms, the transformations of readily biodegradable substrates S_S (not fermentation results, S_A) occur in PHA storage.

Several other sections are illustrated in Bio-P. These were all developed from ASM2d model (Henze et al., 1999). These sections include 1) inorganic soluble phosphorous S_{PO4} , 2) phosphorous accumulating organism X_{PAO} , 3) cell-internal storage product of PAOs X_{PHA} , and 4) polyphosphate X_{PP} . The PHA storage reactions for EAWAG Bio-P employ S_S , whereas ASM2d employs S_A .

The interpretation of these models is related to denitrification through the use of phosphate accumulating organisms (PAOs). The preceding situation is highly significant, as not all the characteristics of the models may be explained completely. The majority of the findings in this work will relate to phosphorous and nitrogen removal.

The availability of models accounting for the EBPR process has increased in the last 20 years. In their study, Filipe and Daigger (1998) identified three models to describe PAOs' anaerobic/aerobic behaviour. These included:

- Model of Wentzel et al. (1989).
- Activated Sludge Model No. 2 (ASM2) (Henze et al., 1995a).

As Barker and Dold (1997) and Henze et al. (1999) explained, these models underwent modifications to take account of denitrifying PAOs. Figure 2.14 illustrates the development of the most important intricate activated sludge models, as identified by Makinia (2010).

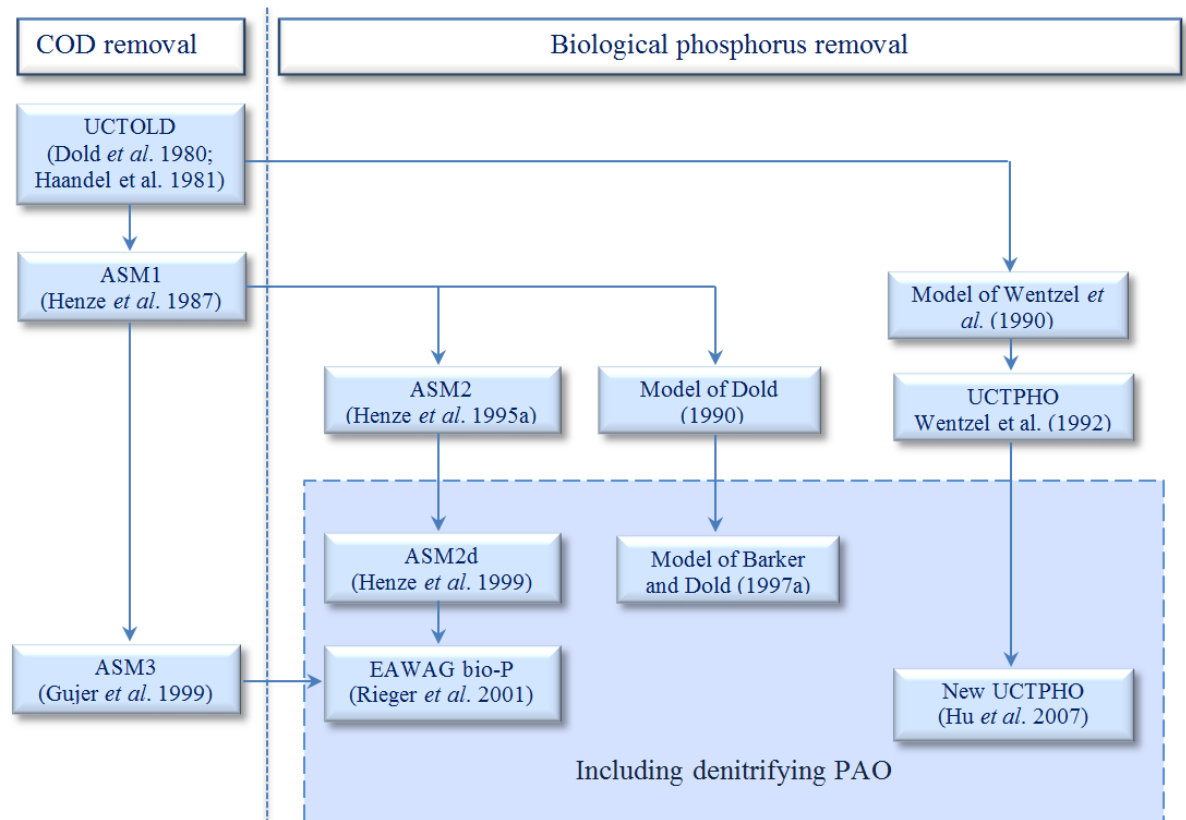


Figure 2.14: Development of the biokinetic model for an activated sludge system.

2.5.2 State-of-the-art in removal of biological phosphorous

Several studies of activated sludge processes have verified that PAOs can use nitrate as an electron acceptor in the absence of oxygen. Nevertheless, it is somewhat unclear whether the same organisms are responsible for the removal of phosphorus at both the aerobic and anoxic stages.

A small growth sludge biomass was observed during aeration, when a high DO concentration was coupled with low sludge loadings. Janczukowicz (2000) reckons that

sludge disposal may be of paramount importance, owing to the production of a small surplus of sludge, as well as its initial stabilisation in the reactor.

In order to obtain phosphorous-rich biomass from a biofilm system, back-washing of filters must take place when the level of internal stored phosphorous in the bacteria is elevated. Limited net phosphorous removal is achieved by guaranteeing limited sludge wasting; frequent wasting can disrupt the performance of the system (Zheng and Long, 2008).

Absence of an electron acceptor in the initial phase could be beneficial for those organisms responsible in the treatment plant. Energy requiring the uptake of fatty acids can be drawn from poly-Ps, and these can then be stored as polyhydroxybutyrate within the cell. In the subsequent phase, oxygen is made available, thus facilitating the growth of organisms on the internally stored substrate, and the accumulation of anaerobically released phosphorous. Kuba (1997) explains that this leads to the sequestration of the substrate from other heterotrophic bacteria, thereby out-competing them.

Amassing phosphorous-accumulating organisms (PAOs) incorporated with biofilm, requires a regulated system. Such a system requires unaerated/aerated conditions in a temporal sequence, under continuous or discontinuous flow, subject to the availability of a substrate under anaerobic conditions. In these conditions, the easily biodegradable substrate is swiftly utilised by PAOs, and then stored in the form of polyhydroxyalkanoates, in association with phosphate degradation, followed by phosphorous release (Zheng and Long, 2008). In aerobic conditions, however, these organisms utilise phosphate from the bulk, thereby increasing intracellular

polyphosphate levels, while using anaerobically stored polyhydroxyalkanoates as a source of carbon and energy.

During the anaerobic phase, phosphate accumulating organisms (PAO) should take up all influent COD, to make sure that no competition is posed by non-phosphorous heterotrophic bacteria that amass in phosphorous. As a corollary, it is possible to have a low summed COD-loading rate during the process, despite having a high rate of anaerobic COD-loading. Overall, for total removal of phosphate to be achieved, there must be a high COD to phosphate ratio in the influent. Adequate ammonium is required for the denitrification of phosphate by phosphate-accumulating bacteria (DPB). Based on these influent quality criteria, Helness (2007) argues that tuning the SBR-cycle is imperative.

Peng (2011), however, states that a distinct improvement in phosphorous removal aptitude was observed after progressively adapting the microorganism communities (PAOs or DNPAOs) to the intermittent anaerobic/anoxic operation model. Based on the findings, the nitrate conveyed by the internal recycle led to a slight weakening of the phosphorous removal aptitude. Accordingly, Peng (2011) contends that it is imperative to adopt an appropriate recycle ratio, to balance the anaerobic zones' microorganism population and nitrate concentrations.

Helness (2001) notes, that on one hand, a low rate of anaerobic COD-loading is required to ensure that no competition is posed by non-phosphorous heterotrophic bacteria that amass phosphorous, while on the other hand, a high rate of total COD-loading is required to allow adequate PHA for phosphate uptake and sufficient biomass net growth.

Significant efforts have been embarked upon to develop a mathematical model to define the EBPR process. According to Wentzel and Ekama (1997), three fundamental microorganism groups must be considered in activated sludge systems models designed to describe biological processes such as nitrification, denitrification, and EBPR. These include: heterotrophic organisms that do not wield the ability to amass polyphosphate (poly -P) (usually referred to as “ordinary” heterotrophs), (2) heterotrophic organisms that wield the ability to amass poly-P (generally referred to as PAOs), and (3) autotrophic organisms responsible for mediating nitrification (usually referred to as autotrophs or nitrifiers). Makinia (2010) notes that the approach espoused by Wentzel and Ekama (1997), and Barker and Dold (1997) does not account for cell internal glycogen conversions, which several researchers have identified as of paramount importance to PAO metabolism. Table 2.1 illustrates these groups’ functions in different oxic conditions.

The prevention of competition, caused by non bio-P aerobic heterotrophs, is imperative in realising effective anaerobic COD removal (Helness and Ødegaard, 2001).

Table 2.1: Principle organism groups for activated sludge system (Wentzel and Ekama, 1997).

Organism group	Principal biological processes	Conditions
Ordinary heterotrophs (unable to accumulate poly-p)	COD removal (organic degradation; oxygen uptake)	Aerobic
	Ammonification (organic N→ NH_4^+)	Anaerobic/Anoxic/Aerobic
	Denitrification (organic degradation, $NO_3^- \rightarrow NO_2^- \rightarrow N_2$)	Anoxic
	Fermentation (fermentable rapidly biodegradable RBCOD→VFA)	Anaerobic

PAOs (heterotrophs) able to accumulate poly-P)	P release (VFA uptake; PHA storage)	Anaerobic
	P release (VFA uptake; PHA storage)	Anoxic
	P uptake (PHA degradation; denitrification)	Anoxic
	P uptake; P removal (PHA degradation; oxygen uptake)	Aerobic
Autotrophs (nitrifiers)	Nitrification ($NH_4^+ \rightarrow NO_2^- \rightarrow NO_3^-$, oxygen uptake)	Aerobic

2.5.3 Sequence batch reactors

There was a re-emergence of concern regarding the use of batch reactors during the 1970s, because of the flexibility provided by small equipment, which is now referred to as a sequencing batch reactor (SBR). The SBR is widely used in wastewater treatment (Grady Jr et al., 2012), and has extended the popularity of wastewater treatment globally.

With respect to the economy of airflow in SBR reactors, it is better to operate the system under conditions of low DO. However, because the concentration of DO can affect multiple factors, the DO concentration and presence or absence of anoxic conditions is identified as having an effect on most microorganisms; this, in turn, can impact biomass deposition and efficiency (Baillod, 1988). Consequently, building a controller that can retain the concentration of oxygen at the desired level is an important issue. PID controller has been taken into account for use in the simulated SBR system to retain the desired value of oxygen (1.5-2.0 mg/l).

In terms of the determination of kinetic parameters, and the SBR nitrification reaction, Münch, (1996) utilised the Monod type of kinetic expression to revise the relationship between nitrification rates and DO concentrations in SBR systems and attributed the range of $K_{O,A}$ from 0.3 - 2 mg/l , which depends on floc size, density and the prevalence of oxygen inside the floc.

$$r_N = r_{N,max} \frac{DO}{DO + K_{O,A}} \quad 2.7$$

r_N = rate of nitrification.

$K_{O,A}$ = oxygen half-saturation coefficient for autotrophic nitrifying bacteria.

$r_{N,max}$ = maximum rate of nitrification.

With regard to SBR biomass, the anoxic P-uptake rate, with nitrite as the electron acceptor, is higher than the rate with nitrate as the electron acceptor. This consideration indicates a particular group of PAO organisms that use nitrite as an electron acceptor in SBR reactors; thus, the DPAOs can make use of nitrate or oxygen as an electron acceptor, while the non-DPAOs can only use oxygen. In addition, DPAO can take advantage of nitrite as an electron acceptor, although it could have a chilling effect on the aerobic P-uptake (Sin et al., 2008).

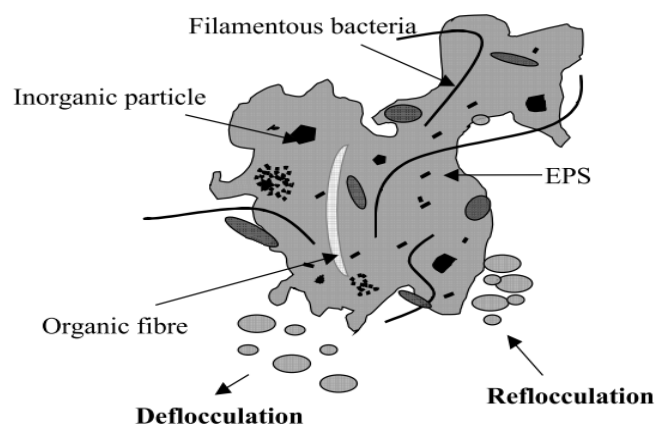
Conversely, due to changes that occur with nitrates and soluble COD in a complete cycle, the SBR reactor can simultaneously accommodate several process functions, such as nitrification, denitrification and P-removal (Zeng et al., 2005).

2.5.4 Activated sludge floc processes

The bulk liquid and floc phase reactions occur in the aerator, and metabolic reactions are accompanied by mass transfer within the floc matrix, thereby establishing a concentration gradient inside the floc, which could have a significant effect on system reaction rates (Tyagi et al., 1996). In addition, the microbial flocs that exist in an aerobic reactor are subject to size distribution which can span three to four orders of magnitude (Li and Ganczarczyk, 1993), affecting both physical and chemical phenomena such as flocculation, substrate transfer, utilisation, and the overall reaction pattern.

Activated sludge flocs consist of a combination (see Figure 2.15) of different bacteria, defunct cells, organic and inorganic components, and extracellular polymeric substances (EPS) (Govoreanu, 2004).

Figure 2.15: Schematic representation of an activated sludge floc



An extensive body of research has focused on modelling the activated sludge process in reference to developing carbonaceous oxidation dynamics, as well as on characterising dissolved oxygen behaviour during the stages of nitrification. Microbial flocs have also been emphasised in many studies (Mustafa et al., 2009).

In terms of flocculation, the general concept of the aggregation of bacteria in a system of sewage treatment can be said to be essential for biomass separation during liquid waste treatment. Additionally, the best measure is an optical technique involving the appearance of the floc, as well as the clarification of water. At the end of the flocculation, the paddle is disconnected and the floc settlement and condensation capacity is examined. During settling tests, there is sometimes an inaccurate indication of floc behaviour; therefore, this test should be performed using a small amount (1 litre) of liquid for experimental measurement (Russell, 2006).

With regard to the floc sizes in the reactor, the flocs in an aeration tank cannot be uniform in size, due to variable surface resistance and degradation along the surface. However, microbial flocs could be associated with a definite type of size distribution across three to four groups in an amount (Li and Ganczarczyk, 1991).

Moreover, floc sizes differ, which could influence the modelling of the overall reaction (Tyagi et al., 1996). Consequently, it is important to take into account the specifications of the secondary clarifier because of the presence of bulking sludge, with poor settling properties. The floc cannot be compacted effectively, leading to the discharge of floc particles into the clarified effluent (Tchobanoglous et al., 2003).

Liao et al. (2006) performed an investigation of the effect of cyclic operation on the allocation and morphology of a floc size at different SRTs using efficient laboratory-scale SBRs. The results indicated a design for SRT (9-12d) because of transitions in floc properties. This SRT maintains a relatively stable microbial community for effective biomass flocculation.

CHAPTER 3

3. METHODOLOGY AND MODEL IMPLEMENTATION

3.1 Methodology

3.1.1 Mathematical Models

For a biological nutrient model to be useful, it needs to have the ability to simulate the metabolic processes exhibited by microorganisms when subjected to aerobic, anaerobic and anoxic conditions. In this particular study, ASM2d was used as it can model nitrogen, and organic and phosphorous substrates when subjected to the aforementioned conditions (Grady Jr et al., 2012).

Notably, the ASM1 is favoured for the modelling of nitrification-denitrification processes. Whereas, the ASM2 is applicable for simulating the utilisation of phosphorous by phosphorous accumulating organisms (PAOs) when subject to aerobic conditions only. By contrast, ASM2d can model the uptake of phosphorous under aerobic and anoxic conditions. As stated previously, ASM2d was developed to express the modelling of phosphorous removal as an extension to ASM2.

Forecasting and modelling can be done using the ASM2d model and associated reactions. The modelling of ASM2d can be used to understand the influences of dissolved oxygen (DO) on the biological nutrient removal of an organism in a sequencing batch reactor (SBR) process (Zhang et al., 2006, Pin et al., 2009). The variations in the amounts of COD, N and P can be predicted by the temporal processing of each step comprising the SBR process.

3.1.2 Solving Non-linear Equations

The only forms of Partial Differential Equations PDEs with analytical solutions are simple ones defined in simple geometrical domains. The majority of nonlinear PDEs do not offer analytical solutions. Consequently, in a bid to compute a suitably approximate solution, an appropriate computational or numerical method is needed.

The development of increasingly powerful computers has rendered numerical methods ubiquitous. Various categories of numerical methods can be used to solve PDEs. These include finite element methods, finite difference methods, and boundary element methods. These aim to solve both linear and nonlinear PDEs comprehensively.

The collocation method is a category of numerical methods that can be comprehensively used to solve the aforementioned equations. One of its advantages is that the collocation method is regarded as the method of choice to resolve ODE problems that are complex and difficult.

The orthogonal collocation method converted differential equations into a group of algebraic equations, which can be solved using an external nonlinear solver. This collocation method estimates a differential equations' solution through the linear integration of basic functions, established by requiring that the ODE be satisfied at a discrete set of mesh points. Satisfaction of the boundary conditions is also required. Thereafter, in terms of solving algebraic equations, the Newton-Raphson method will be utilised.

3.1.3 SIMBA software

SIMBA is a simulation system constituted of versatile software useful not only for modelling but also in dynamic simulations relating to the wastewater-engineering field. The basis of SIMBA is both Simulink and MATLAB, which enable it to fulfil most of the common needs relating to the simulation of wastewater processes. In extending both Matlab and Simulink, SIMBA applies block libraries and chemical and biological treatment processes. The control window of SIMBA and a sample block library for SIMBA are shown in Figure 3.1.

Notably, the applicable mathematical models constitute tools suitable for calculating and studying a system's evolution. Fundamentally, various partial differential or non-linear ordinary equations have been utilised for mathematical models that are applicable to environmental systems. There is a recognised need to simplify actual processes that contain the practical model parameters of mathematical models. Moreover, ASM2d entails one such model; using non-linear ordinary equations to describe the metabolism of various microorganisms. Thus, it is possible to employ SIMBA, to simulate an organisms' metabolism so that it is applicable to the ASM2d model.

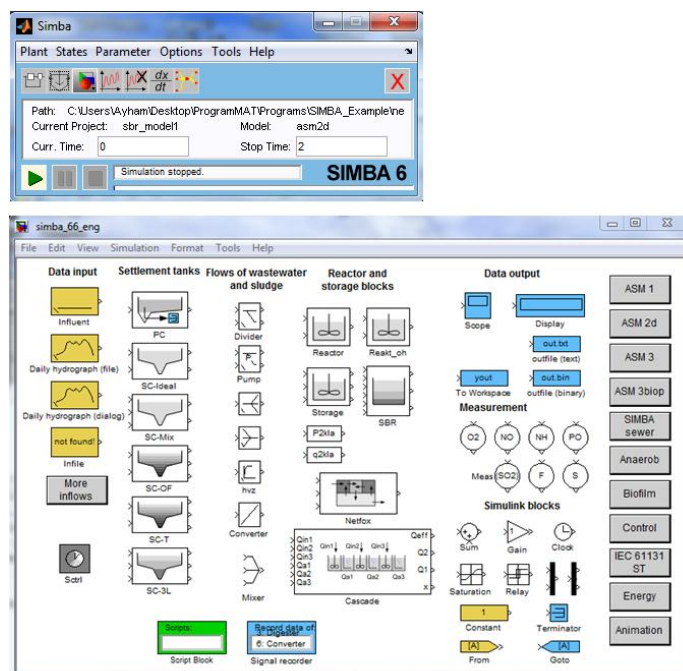


Figure 3.1: SIMBA control window and block library

3.1.4 Installation characteristics

- Wastewater

Warsaw University of Technology provided the wastewater influent utilised in this study. It was characterised by 352–867 gO_2m^{-3} chemical oxygen demand (COD), 49.17–164 $gCODm^{-3}$ total Kjeldahl nitrogen (TKN), 10–23.87 gPm^{-3} total phosphorous (TP), 0.2–2 gNm^{-3} ammonia-nitrogen ($NH_4^+ - N$), 0.1–1.5 gNm^{-3} nitrate nitrogen ($NO_3 - N$). Additionally, in the mixed liquor, the suspended solids (MLSS) of activated sludge were 6000–8000 gm^{-3} , the level of pH was about 7.0, and the temperature is 20°C.

- Reactor operation

The schematic installation of the equipment used in the model experiment is depicted in Figure 3.2. This study was carried out in a SBR reactor, with 30 l, 0.03 m^3 volumes, a height diameter of 0.5m and a 0.06 m^2 cross area. In terms of reaction input, the plant was operated for 60 days, with three cycles per day; each cycle had seven periods, as shown in Figure 3.3. In addition, the reactor was supplied with wastewater influent, which had been converted into model vectors (ASM2d). In all simulations, the dissolved oxygen concentration in the bulk was maintained at a constant level of 1.7 gm^{-3} during the aerobic phase. The temperature is 20°C. The initial mixed liquor suspended solids (MLSS) of the activated sludge was 3000 gm^{-3} .

After the settling period, about 5 l of supernatant were discharged from the top of the reactor, and replaced with 5 l of domestic wastewater during the first and second fills. The amount of substrate withdrawn was 600 ml of excess sludge every cycle, and, this

was replaced with 600 ml of domestic wastewater; thereby ensuring a sludge retention time (SRT) of approximately 10 days. This operation enabled a mixed liquor suspended solid (MLSS) concentration of activated sludge of approximately $6000\text{--}8000\text{gm}^{-3}$. Moreover, the reactor influent and effluent values were measured every day for 60 days.

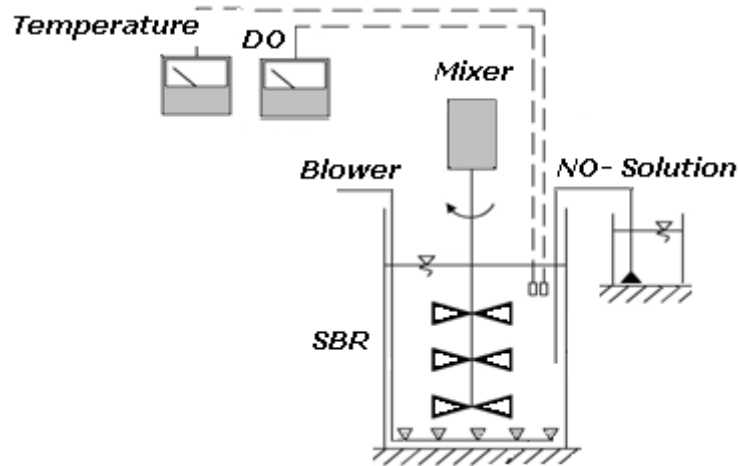


Figure 3.2: Schematic representation of the laboratory apparatus

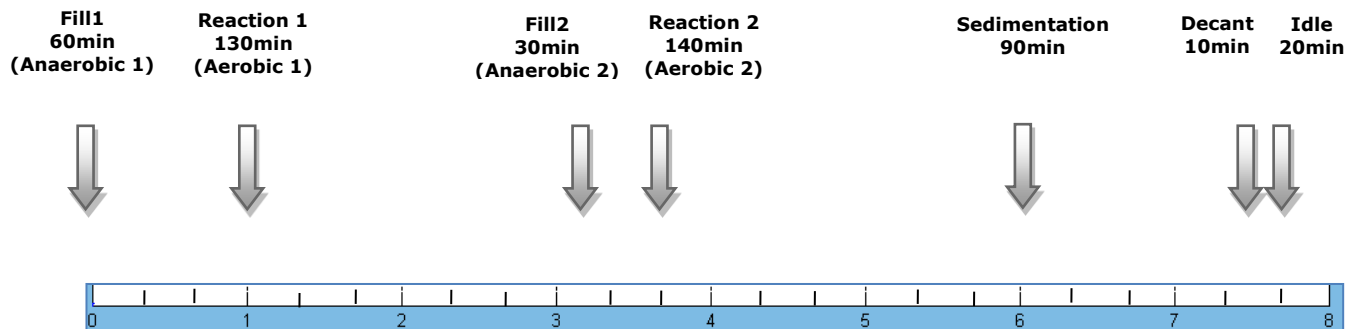


Figure 3.3: SBR cycle definition during one period (8 hours)

3.1.5 Simulated systems

The model process is typically represented using a simulated diagram (see Figure 3.4) divided into an influent model, a process and a feedback controller. The influent model consists of the variable converter and input reaction stages, and the process involves the SBR reactor. Although there is no feedback (returned sludge) in this process, it is important to consider the feedback controller for the input reaction; such as control in the blender, period of time, pumps and airflow.

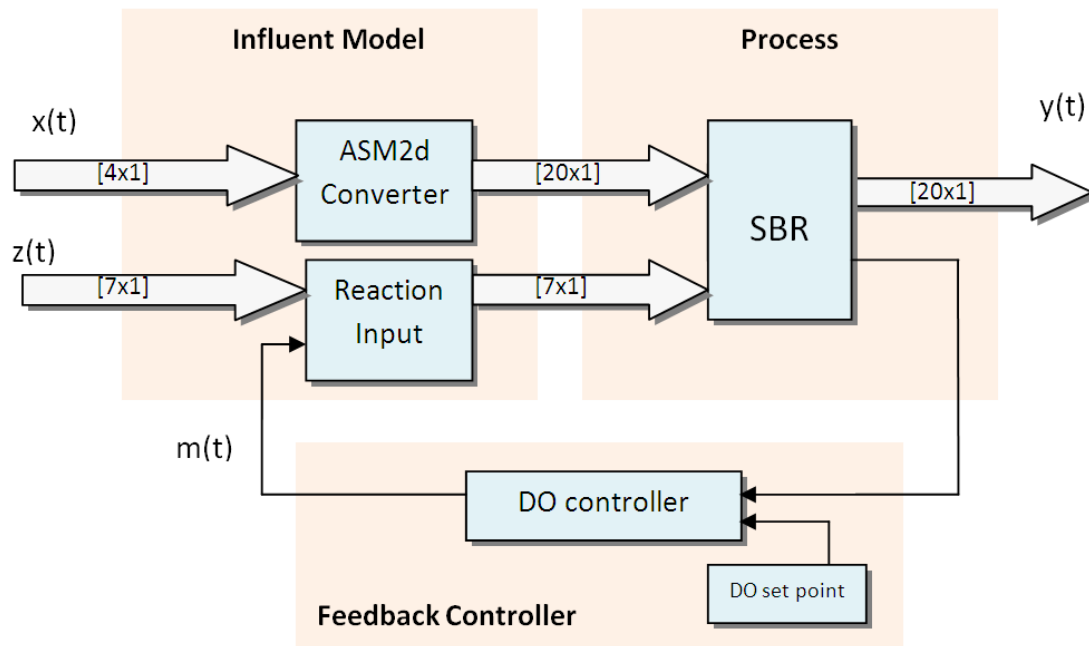


Figure 3.4: Structure of a SBR with ASM2d model

$x(t)$: Input Variables (inflow).

$z(t)$: Input Variables (timer and gain).

$y(t)$: Output Variables (outflow).

$m(t)$: Manipulated Variable.

3.1.6 Simulation Model

The simulation model in this study is based on the ASM2d; the model was successfully applied in simulations of the biological removal of nitrogen and phosphorous. All the simulations were implemented in SIMBA, a dedicated software package for modelling and simulating wastewater treatment processes for biological wastewater.

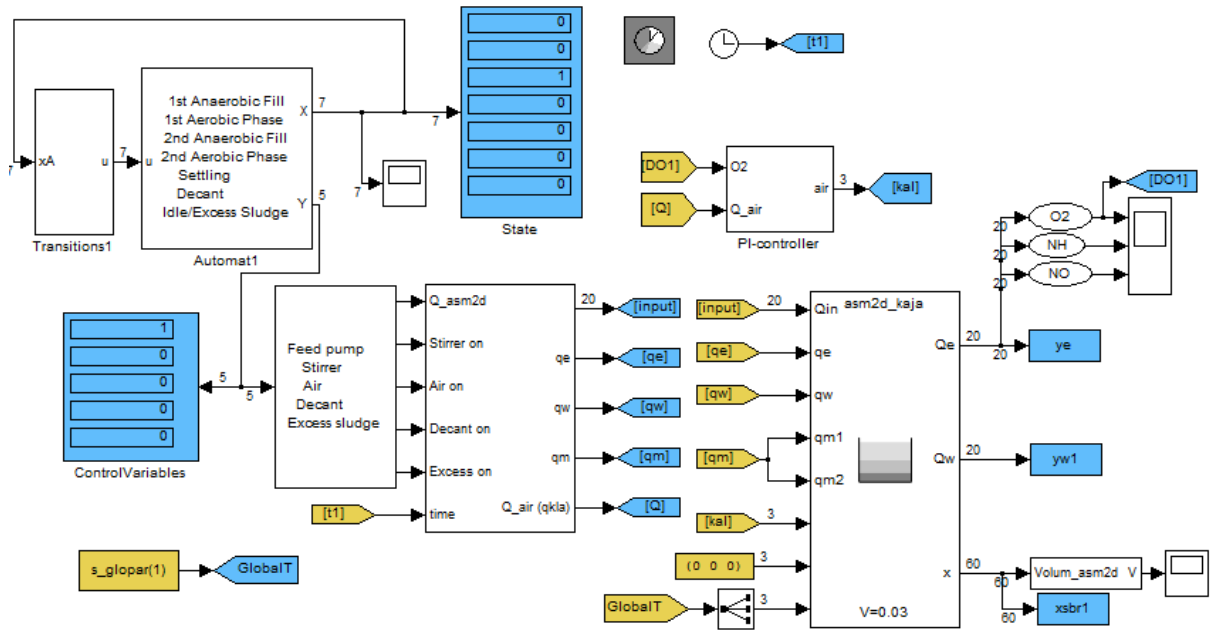


Figure 3.5: SIMULINK system construction of SBR with ASM2d model.

3.2 Extension of ASM2d with the floc model

ASM2d was developed by extending and integrating concepts from Henze's et al. (1995) ASM2 and Henze's et al. (1987) ASM1. ASM2's drawback was fixed by the development of ASM2d. The ASM2 was developed by extending the concepts of ASM1. ASM2 is more intricate intricacy and takes more components related to wastewater and activated sludge into account. ASM2 also integrates supplementary biological processes, that have been put in place to enable the biological removal of phosphorous. ASM2d was developed by slightly extending ASM2.

For optimum processing, it is essential that dissolved oxygen content remains above 1.5 mg/l. ASM2d was used to model the data gathered using an initial investigation, and to increase the efficiency of WWTPs (Pin et al., 2009).

3.2.1 Limitations and proposed modification for ASM2d

The most significant limitations of ASM2d, as identified by Henze et al. (2000), include:

- The validity of the model is limited to municipal wastewater. For the model to be used outside these limits Ky et al. (2000) recommend that specific rate equations should be incorporated when accounting for any additional reactions that may occur (Baetens, 2001).
- During the aeration phase, it is impossible to model processes with acetate overflow. Brdjanovic (1998) provided a proposal to counter this limitation.
- pH is supposed to be close to neutral.
- A temperature range of 10-25°C should be observed.

3.2.2 Model components

In activated sludge models, there is a distinction between soluble and particulate components. S is used to denote soluble components, and X to denote particulate components. There is an assumption that suspended components relate to the activated sludge, and that concentration can occur during the settler stage. Soluble components typically dissolve in the wastewater that transports them. Filtration does not necessarily separate soluble and particulate components. Analysis of some components requires bioassays as a result of their interactions with biomass. Electrical neutrality (no ionic charges) is required in particulate model components, not in soluble components.

During the removal of carbon and nitrogen, the only bacteria taken into account are heterotrophic bacteria (previously X_{BH} currently X_H) and autotrophic bacteria (previously X_{BH} currently X_{AUT}). The establishment of the biological removal of phosphorous, led to the introduction of separate biomass, X_{PAO} , and internal storage components, i.e. a lump sum of organic storage components as PHAs (X_{PHA}) and poly-phosphate (X_{PP}).

Barker and Dold (1997) extended the model for the biological removal of phosphorous, by making a model capable of removing denitrifying phosphorous. The Wentzel-model, which had presented adequate experimental evidence, facilitated the incorporation of this reaction into the general model. Similar to ASM2d, Barker and Dold's (1997) model also assumed that some PAOs can utilise nitrate as an electron acceptor. Barker and Dold, however, suggested that the stored poly-phosphate content should be divided into ones to be released and the ones to be fixed.

When defining ASM2d components, they are divided into soluble (S) and particulate (X). It has been assumed that particulate components are associated with the activated sludge, which can be concentrated by a clarifier tank (sedimentation), and the soluble components can only be decanted with water. Table 3.1 provides a short definition of the dissolved and Particulate Components of ASM2d model.

Table 3.1: Activated sludge model ASM2d components (Henze et al., 1999).

Component	Definition	Units
Dissolved Components		
S_{O_2}	Dissolved oxygen	$gO_2 m^{-3}$
S_F	Readily biodegradable organic substrate	$gCOD m^{-3}$
S_A	Fermentation products (acetate)	$gCOD m^{-3}$
S_{NH_4}	Ammonium plus ammonia nitrogen	$gN m^{-3}$
S_{NO_3}	Nitrate plus nitrite nitrogen	$gN m^{-3}$
S_{N_2}	Dinitrogen, N_2	$gN m^{-3}$
S_{PO_4}	Inorganic soluble phosphorous (phosphate)	$gP m^{-3}$
S_I	Inert, non-biodegradable organic	$gCOD m^{-3}$
S_{SALK}	Bicarbonate alkalinity	$mole HCO_3^- m^{-3}$
Particulate Components		
X_I	Inert, non-biodegradable organic	$gCOD m^{-3}$
X_S	Slowly biodegradable organic substrate	$gCOD m^{-3}$
X_H	Heterotrophic organisms	$gCOD m^{-3}$
X_{PAO}	Phosphate-accumulating organisms of PAO	$gCOD m^{-3}$
X_{PP}	Stored Poly-phosphate of PAO	$gP m^{-3}$
X_{PHA}	Organic storage products of PAO	$gCOD m^{-3}$
X_{AUT}	Autotrophic, nitrifying organisms	$gCOD m^{-3}$
X_{TSS}	Particulate material as model component	$g TSS m^{-3}$
X_{MeOH}	Ferric-hydroxide, $Fe(OH)_3$	$g Fe(OH)_4 m^{-3}$
X_{MeP}	Ferric-phosphate, $Fe(PO)_4$	$g Fe(PO)_4 m^{-3}$

3.2.3 Matrix structure

Petersen (1965) was tasked with the responsibility of developing a matrix that would enhance transparency and simple comparisons among different models. The explanation of this structure, and the associated conservation equations, are done using a simple example, which shows how the matrix can be utilised in the definition of fundamental reactions, irrespective of the system configuration (Henze et al., 1999, Henze et al., 1987, Gujer et al., 1995, Henze et al., 2000).

Table 3.2: Process kinetics and stoichiometry for heterotrophic bacterial growth (Henze et al., 2000)

Process j \ Component i	1	2	3	Process Rate ρ_j
	X_B	S_S	S_O	
1 Growth	1	$-1/Y$	$1 - 1/Y$	$\mu \frac{S_S}{K_S + S_S} X_B$
2 Decay	-1		-1	$b X_B$
Conversion Rate $ML^{-3}T^{-1}$	$r_i = \sum v_{j,i} * \rho_j$			μ : Maximum specific growth rate K_S : Half-velocity constant b : Specific decay rate
	Biomass $M(COD)L^{-3}$	Substrate $M(COD)L^{-3}$	Oxygen $M(-COD)L^{-3}$	Y : True growth yield

The above table is an illustration of the matrix structure. The right side show the equation rates for both processes, alongside the kinetic parameters on the bottom right. The table does not provide values for the kinetic and stoichiometric parameters. Separate tables are used for the demonstration of the stoichiometric matrix, and the process rate equations for more intricate models.

To calculate the rate of biomass production for dissolved oxygen S_O , the stoichiometric coefficients $v_{j,i}$ products are added to the process component i 's rate expressions ρ_j and are summed.

$$r_{X_B} = (1 - 1/Y) \cdot \mu \frac{S_S}{K_S + S_S} X_B + (-1) \cdot b X_B \quad 3.1$$

The same concept will be applied for all types of activated sludge models, the transformation process and the components are characterised with the indices i and j . The Stoichiometric matrix, which presents the coefficients $v_{j,i}$, and the rate of production of the component, in all parallel processes will be r_i . This can be calculated from:

$$r_i = \sum v_{j,i} * \rho_j \quad 3.2$$

Where ρ_j is a rate vector over all processes, j (Table A2).

Mathematically, the conservation equations can be defined as the equivalent of the standard in chemical reactions, elements, electrons and electrical charging. The conservation equations, must be equal to zero over all components i , and could be written as:

$$\sum v_{j,i} * i_{c,i} = 0 \quad 3.3$$

Where $i_{c,i}$ is conversion factor to convert the units of components i to material c .

$v_{j,i}$ is stoichiometric coefficient for component i and process j

The conversion factors are shown in table A1. These factors can be calculated from chemical stoichiometry.

For example:

$$i_{COD,5} = -64gO_2/14gNO_3^- \quad \text{from:} \quad NO_3^- + H_2O + 2H^+ \rightarrow NH_4^+ + 2O_2$$

This means that 1 mole of nitrate (14 gN) has a negative oxygen demand of 2 moles of oxygen (64 gO₂). Similarly,

$$i_{COD,9} = -24gO_2/14gN_2 \quad \text{from:} \quad 2N_2 + 6H_2O + 4H^+ \rightarrow 4NH_4^+ + 3O_2$$

3.2.4 Pathways interaction components

Different components, stoichiometry and processes are considered in ASM2d, because these formed complex pathways. Figure (3.6, 7 and 8) depicts the pathways of non-poly-P heterotrophs, poly-P heterotrophs, autotrophs, hydrolysis and fermentation, respectively. The definitions and notations for these components are described in Table 3.1.

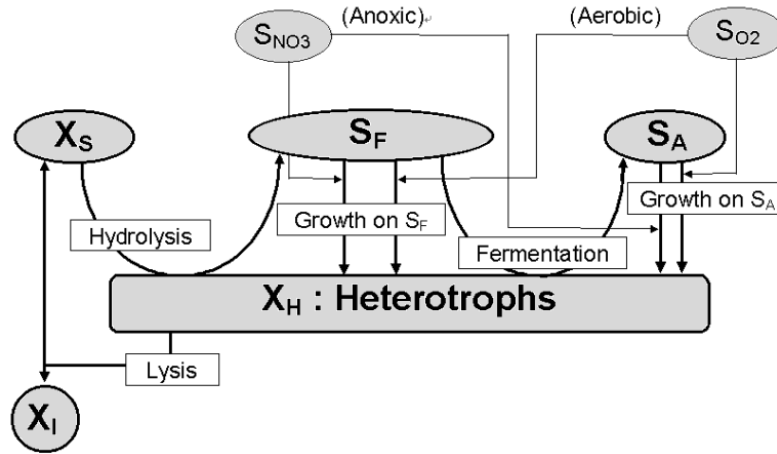


Figure 3.6: Pathway of non-poly-P heterotrophs

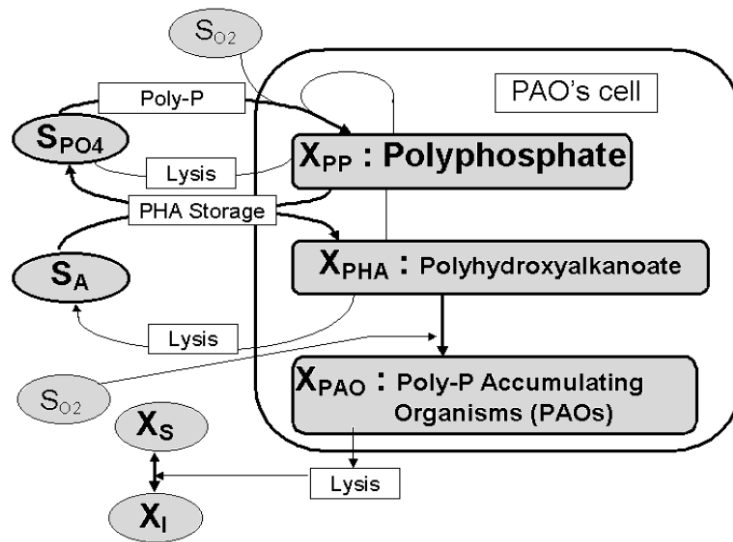


Figure 3.7: Pathway of poly-P heterotrophs

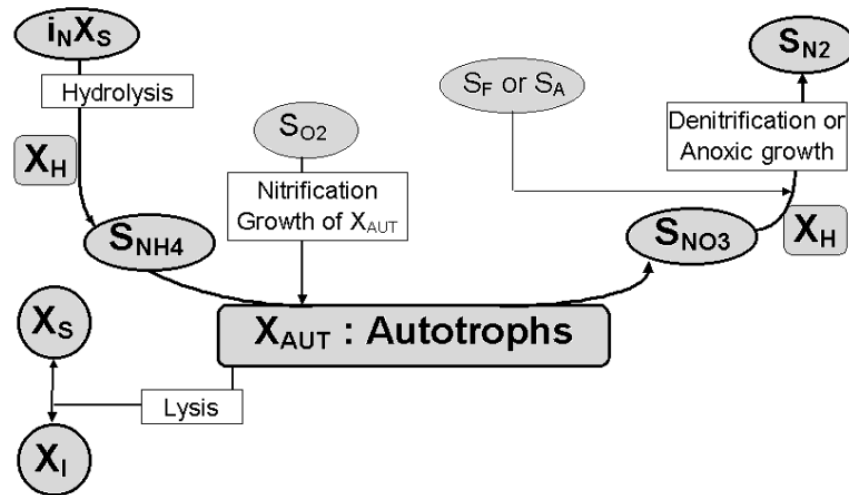


Figure 3.8: Pathway of autotrophs

3.3 Flocculation

3.3.1 Introduction

The purpose of the activated sludge process can be briefly explained as a biological treatment to decrease the biodegradable organic compounds in wastewater. Figure 3.9 represents the biological stage of the activated sludge process. It commences with the influent, which is introduced into the aeration tank, followed by the clarification tank. This material then settles in the form of sludge and some parts of it are returned to the aeration tank.

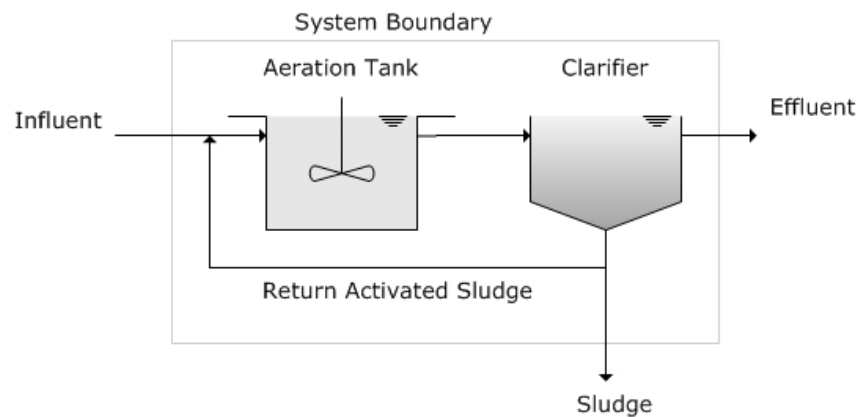


Figure 3.9: The main biological stage of the activated sludge system

This process relies on sewage aeration, and a variety of mixed bacteria, which convert the biological pollution and ultimately enable the formation of biomass, also known as flocs. The microorganisms are more susceptible to certain process factors, such as temperature, pH, and oxygen concentration, than others. The efficiency of the activated sludge process is affected by the capability of the sludge flocs to settle. However, insufficient quantities of a secondary clarifier, to eradicate biomass from the wastewater, could lead to a lack of precision in the efficiency of activated sludge processes.

Regarding the effectiveness factors most related to the implementation of the activated sludge with floc assumption, there are two that inform the carbon oxidation and nitrification process. These factors make the system more receptive to the changes in floc size. Therefore, to ensure that process controls are more efficient, it is important to consider concept of activated sludge in depth, particularly relative to floc size distribution.

The size and distribution of activated sludge flocs in an aeration tank, including dispersed microorganisms and very small flocs, can fit the power-law model:

$$f(x) = \alpha x^{-\beta} \quad 3.4$$

Where $f(x)$ is the power-law density function, x is floc size, and α and β are the distribution parameters. As a parameter α can be presented as the factor of the total amount of flocs in mixed liquid volume, the parameter β can also relate to the flocs in several size groups.

Li and Ganczarczyk (1993) found that only a change in floc size distribution directly affects dissolved oxygen. According to the previous equation, there is a correlation between dissolved oxygen and the parameter α . It was found that dissolved oxygen responds when the correlation coefficient is equal to -0.26. Whereas, in the case of changing the parameter β , the correlation coefficient β makes no consistent indication regarding the study of dissolved oxygen changes, which means that the correlation coefficient cannot be identified.

On the other hand, several preceding studies have suggested that DO could have a substantial effect on the amount of floc, within several size limits. Nevertheless, these assumptions were not reliable. Li and Ganczarczyk, (1991, 1993) reported that, for a

given level of organic loading, the activated sludge floc size tended to increase as the reading for dissolved oxygen decreased. This is attributed to the growth of filamentous microorganisms, which survive better than bacterial floc in surroundings lacking in oxygen.

With respect to the development of the activated sludge model at low DO, the impact of effectiveness factors on N and P removal has to be considered. For example, in ASM1, these factors correlated with aerobic autotrophy, aerobic heterotrophy and anoxic growth rate (Tyagi et al., 1996).

In the place of MLSS, Mixed liquor volatile suspended solids (MLVSS) can also be used. The level of accuracy when representing the concentrations of biomass is slightly more in MLVSS than MLSS, because MLVSS only counts the organic solids. The units used in the expression of an activated sludge reactor's biological cell concentrations are mg/l of mixed liquor suspended solids (MLSS); i.e. the suspension's agitated biomass.

3.3.2 Flocculation mechanisms

Since slow mixing is one of the attributes of flocculators, they only use tanks that have slowly rotating paddles, or other mixing devices such as baffles, or air bubbles.

Coagulation refers to destabilisation, using particle charge neutralisation and initial aggregation of colloids. The primary aim of coagulation is to bring things together. Coagulation is integrated with flocculation and chemical treatments, as are the requisite processes of precipitation and chemical treatment. Flocculation refers to the agglomeration of coagulated colloidal as well as suspended materials that are finely divided, either using physical mixing or chemical coagulant aids.

Models take account of the size of the particles, the rate of shear, the fluid's dynamic viscosity and collisions per unit of time. However, the predictive aspects of such models are complex and arduous even when compared with the results of a simple jar test. Consequently, they are only useful as research tools. Russell and David (2006) hypothesise that it is hard to predict a floc's size and distribution, as well as the number of collisions. When the reactor has a level of MLSS (around 3000 mg/L) (Wang et al., 2007), the impact of the concentration of biomass on the sludge flocs' flocculating ability and compressibility is reduced.

Several flocculation mechanisms have been developed to explain the formation of sludge floc. The effectiveness of these models is contingent on certain conditions, and unexplained experimental phenomena often pose challenges to their validity. Polymer bridging is currently the most widely accepted mechanism. There is still a shortage of the information regarding cellular hydrophobic interactions. The underlying forces that govern the formation of sludge floc are yet to be clearly identified; particularly the mechanisms for dispersed growth and sludge floc disintegration.

Previous studies have established contradictory conclusions regarding the role of sludge surfaces and operating variables (e.g. SRT) in flocculation (Sin et al., 2006). These contradictory conclusions result from several uncontrollable factors arising among samples of sludge from poorly controlled full-scale activated sludge systems. Becoming acquainted with how the performance of activated sludge processes is impinged on by a specific environmental and operating variables, by creating conditions that are rigorously controlled, can be very advantageous.

Measurement techniques that are reliable and reproducible are of paramount importance. Improvements can still be made to sludge floc measurement techniques. Regardless of several publications that have been made pertaining to the physical and/or chemical properties of sludge flocs, integrated literature is limited. There is ongoing uncertainty regarding the correlation between the physicochemical properties and the compressibility, settleability and flocculating ability of sludge flocs.

Haegeman (2006) explored how the dynamics of bacterial growth impinge on flocculation in a bioreactor. In the context of the activated sludge process, the combining of physicochemical and biological phenomena mostly occurs in a reaction tank.

3.3.3 Aggregation and bioflocculation

Although microbiologists have developed a vast body of literature observing microbial life, studies have largely focused on pure microbial cultures grown in liquid suspension, although most microbial life exists as microbial communities that grow aggregates (Liao et al., 2006). These aggregates can be either biofilms or flocs (planktonic biofilms), connected to each other with extracellular polymeric materials. Prior to the identification of the general ubiquity of microbial aggregates, environmental engineers who recognised them be essential in the treatment of biological wastewater, aimed to exploit them by establishing mixed microbial communities. Related growth processes are dependent on biofilms attached to solid supports, which ensure that microbial communities are retained. On the other hand, the retention of microbial communities in suspended growth processes is facilitated by the generation of floc particles that can be removed through gravity sedimentation, membrane processes, or recycling back into the

bioreactor biofilms. Floc particles appear to be different from a macroscopic point of view; however, at the microscopic scale, a myriad of similar attributes and similar mechanisms are implicated in their formation.

3.3.4 Floc formation and single floc size

The growth of numerous species of natural bacteria in activated sludge processes necessitates floc formation, owing to the use of gravity clarifiers. Floc formation takes place at lower rates of growth, and at lower nutrient levels, i.e. in starvation or stationary growth conditions.

With regard to dissolved oxygen, the actual concentration of DO in biological flocs is less than that measured in the bulk solution, because oxygen permeates into the flocs.

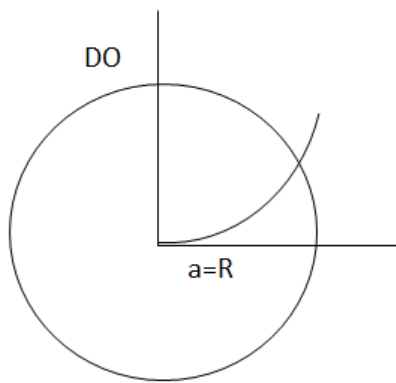
When evaluating the effectiveness factors, the gradient of dissolved oxygen concentration within the flocs was taken into account in the same manner as Wang (2006), while the concentrations of other components were assumed to correspond equally to their concentrations in the bulk phase. As shown in the illustration in Figure 2.6, the activated sludge floc was expected to be spherical, and it was assumed that the oxygen would be dissolved and transferred from its exterior to the core. Molecular dispersion, motivated by the concentration gradient is the main assumption informing the transportation of oxygen.

Assumptions were made regarding, the uniform distribution of microbes within the floc, the oxygen consumption, and the oxygen dispersion. The entire process is in a state of equilibrium when there is stability in the rate of oxygen consumption; dispersion within the floc would then lead to either oxygen's absolute penetration, or its depletion. In the

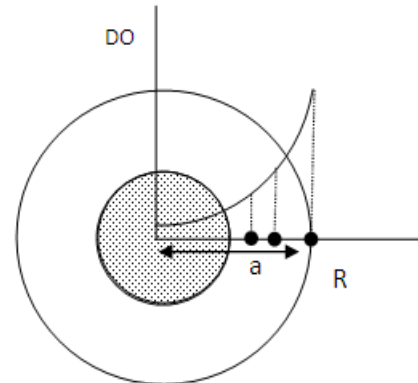
case of the former (Figure 3.10, left panel), no anoxic zone would be produced in the floc, and thus nitrate could not be converted to nitrogen gas, but the aerobic reaction rates such as nitrification and organic degradation would decrease. In the case of the latter (Figure 3.10, right panel), there would be formation of an anoxic zone in the floc core, and thus denitrification would occur, and the aerobic reaction rates would consequently decrease.

In the present case, however, the changes in COD concentration did not significantly affect nitrogen removal as they had done in the conventional denitrification processes.

In contrast, the DO had a dominant effect on the nitrogen removal.



(a): DO concentration within a bio-floc



(b): Illustration of aerobic and anoxic zones

Figure 3.10: Diagram of an activated sludge floc

In the case of nitrogen removal, the zone inside a single-sludge floc can be described in terms of an aerobic and anoxic region, as exemplified in Figure 3.10(b).

The equilibrium will be achieved when the rate of oxygen consumption is equal to that of the spreading within the floc, which also leads to complete diffusion or exhaustion of the oxygen.

As mentioned previously, when a reaction takes place, one of two possible phenomena can occur:

- 1- Oxygen completely penetrates the entire floc with the highest concentration at the surface, and lowest but non-zero concentration at the centre.
- 2- Oxygen distributes on the outer layer of the floc when an anoxic core is present.

Mass balances for microorganisms and limiting substrate under steady-state conditions can be considered as the following expressions:

$$w(S_i - S) - R_S = 0 \quad 3.5$$

Where w is the dilution rate (d^{-1}), and (S_i, S) the input and output substrate concentrations ($gCODm^{-3}$) respectively, and R_S , the rate of substrate consumption ($gCODm^{-3}d^{-1}$).

3.3.5 Mathematical equations of oxygen gradient within a single floc

As illustrated in the model below, the physical and chemical process of mass transfer is contingent on the diffusion and the radial distance:

$$\frac{\partial C}{\partial t} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{2}{R} \frac{\partial C}{\partial x} \right) + \text{reaction rate} \quad (0 \leq x \leq R) \quad 3.6$$

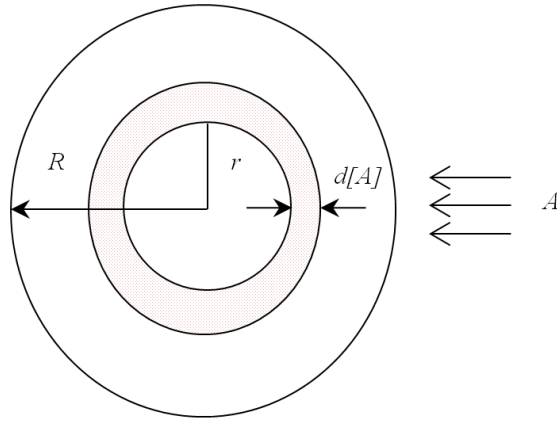


Figure 3.11: A differential element of a spherical pellet

A simple first-order reaction: ($A \rightarrow \text{Products}$) occurs when explaining first-order isothermal reactions in a spherical catalyst

$-r_A = k_v[A]$ is an expression of a first-order rate, which takes place in a spherical catalyst pellet, as illustrated in Figure 3.11. For convenience, the rates are based on the catalyst volume, instead of the weight. According to Doraiswamy (2013), the equation that should be used in the selection of appropriate continuity for spherical coordinates is as follows:

$$0 = D_A \left(\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial [A]}{\partial r} \right) \right) + r_A \quad 3.7$$

To attain an equation for the first-order reaction, the equation is rearranged to become:

$$D_A \left(\frac{\partial^2 [A]}{\partial r^2} + \frac{2}{r} \frac{\partial [A]}{\partial r} \right) = k_v [A] \quad 3.8$$

C represents the concentration of the variable, D represents the dispersion coefficient, and the radial distance.

By specifying the boundary conditions, a solution for the equation can be found:

$$[A] = [A]_S \quad (\text{Surface})$$

$$\frac{d[A]}{dt} = 0 \quad (\text{Centre})$$

An assumption has been made that the sphere illustrated in figure 3.11, a is a floc. The balancing mathematical equation for the concentration of oxygen S_o with the distance a from the floc becomes:

$$\frac{\partial S_o}{\partial t} = D \left(\frac{\partial^2 S_o}{\partial a^2} + \frac{2}{a} \frac{\partial S_o}{\partial a} \right) + r_i \quad 3.9$$

r_i represents the rate at which a component, i , is produced (see Eq. (3.2)).

The boundary conditions refer to the concentration at the floc's centre:

$$\frac{\partial S_o}{\partial t} = 0 \quad \text{at} \quad a = 0 \quad 3.10$$

The concentration on the superficies is:

$$S_o = S_o^b \quad \text{at} \quad a = R \quad 3.11$$

The solutions for Equations 3.9 and 3.11 are obtained using the orthogonal collocation algorithm at i th, and are transformed as:

$$\frac{\partial S_{o,i}}{\partial a} = \left(\frac{1}{R} \right) \left(\frac{\partial S_{o,i}}{\partial l} \right) = \frac{1}{R} \sum_{k=1}^{m+2} A_{i,k} * S_{o,k} \quad 3.12$$

$$\frac{\partial^2 S_{o,i}}{\partial a^2} = \left(\frac{1}{R^2} \right) \left(\frac{\partial^2 S_{o,i}}{\partial l^2} \right) = \frac{1}{R^2} \sum_{k=1}^{m+2} B_{i,k} * S_{o,k} \quad 3.13$$

Where $(l = a/R, 0 \leq l \leq 1)$ is the normalised distance, and m is the number of collocation points. A, B are orthogonal collocation matrices for the first and second order derivatives respectively.

When compensating for both Equations 3.12 and 3.13 in the Equation 3.9:

$$\frac{\partial S_o}{\partial t} = \frac{D}{R^2} \left(\sum_{k=1}^{m+2} B_{i,k} * S_{o,k} + \frac{2}{l} * \sum_{k=1}^{m+2} A_{i,k} * S_{o,k} \right) + r_i \quad 3.14$$

3.3.6 Effectiveness factors of a single floc

Microorganisms exist everywhere, and an enormous variety of microorganisms could be found in the nitrogen and phosphorous removal system. The reaction mechanism cannot be concealed from complications because of the coexistence of competitive behaviours among microorganisms. In order to lessen the said complexity, the IAWQ Task Group recommends that only three groups of microorganisms should survive in this kind of system, representing organic matter by heterotrophs, nitrogen and phosphorous removal, by the autotrophs and PAOs respectively. Furthermore, ASM2 described the reaction kinetics of these microorganisms, to assist in the elaboration of their removal characteristics. However, the major limitation of ASM2d is that the filamentous growth of biomass growth and bulking of sludge cannot be described using this model. Therefore, this section will describe how ASM2d model can be extended in terms of floc size effect.

When the model works at low DO concentrations, various kinetic parameters need to be corrected by introducing consequent effectiveness factors, as long as floc size is considered. These parameters relate to the storage rate of polyphosphate ρ_{PP} , the growth rate of phosphorous-accumulating ρ_{PAO} , the nitrifying growth rate of ρ_{AUT} (an autotrophic organism), and the growth rate of heterotrophic organisms on fermentable substrates ρ_F . Moreover, some components will be treated as the dependent variables for chemical oxygen demand (COD) in processes such as hydrolysis (aerobic, anoxic and anaerobic), and with heterotrophic organisms. As a result, the stoichiometric and composition matrices take on a new form within the adapted parameters.

In contrast, effectiveness factors will be derived according to the relationship between dissolved oxygen and the radial distance of the floc. The system's overall effectiveness factors will then be determined.

According to the ASM2d model, the total COD includes the following components:

$$COD = S_A + S_F + S_I + X_I + X_S + X_H + X_{PAO} + X_{PHA} + X_{AUT} \quad 3.15$$

This equation describes the effects of the parameters that should be modified on COD.

Slow biodegradable substrates X_S have a heavy molecular weight, and particulate organic substrates must be subjected to external cell hydrolysis before degradation; the outcome of hydrolysis will involve fermentable biodegradable organic substrates S_F , which can be used for heterotrophic growth. Although it is assumed that organic substrates S_F can serve as substrates for fermentation, they comprise no fermentation products S_A , and so must be modelled separately from soluble organic components. As Figure 4.7 shows, during the slow biodegradable process, biodegradable organic substrates S_F can be used for heterotrophic growth, and fermentation products S_A can be used for the growth of both heterotrophs and PAOs.

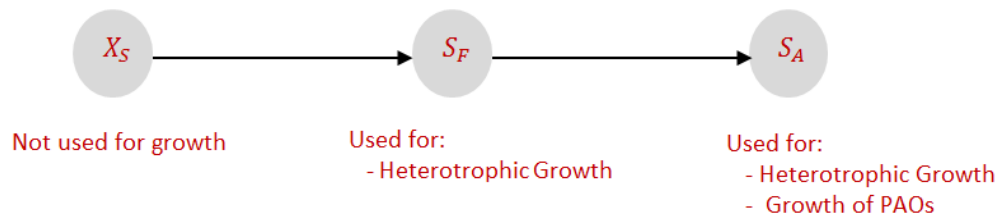


Figure 3.12: Pathway of hydrolysis and fermentation

$$\rho'_{14} = \mu_H \cdot \frac{S_{O2}}{K_{HO2} + S_{O2}} \cdot \frac{S_F}{K_F + S_F} \cdot \frac{S_F}{S_F + S_A} \cdot \frac{S_{NH4}}{K_{HNH4} + S_{NH4}} \cdot \frac{S_{PO4}}{K_P + S_{PO4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H * \rho_F$$

$$\rho'_{11} = q_{PP} \cdot \frac{S_{O2}}{K_{O2} + S_{O2}} \cdot \frac{S_{PO4}}{K_P + S_{PO4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot \frac{K_{MAX} - X_{PP}/X_{PAO}}{K_{PP} + K_{MAX} - X_{PP}/X_{PAO}} X_{PAO} * \rho_{PP}$$

$$\rho'_{13} = \mu_{PAO} \cdot \frac{S_{O2}}{K_{O2} + S_{O2}} \cdot \frac{S_{NH4}}{K_{NH4} + S_{NH4}} \cdot \frac{S_{PO4}}{K_P + S_{PO4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot X_{PAO} * \rho_{PHA}$$

$$\rho'_{18} = \mu_{AUT} \cdot \frac{S_{O2}}{K_{O2} + S_{O2}} \cdot \frac{S_{NH4}}{K_{NH4} + S_{NH4}} \cdot \frac{S_{PO4}}{K_P + S_{PO4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_{AUT} * \rho_{AUT}$$

Where ρ_F , ρ_{PP} , ρ_{PHA} and ρ_{AUT} are effectiness floc factors and the other cooffecients and variables are explained in table (4.1, A4, A5 and A6).

As a result of the addition of effectiveness factors to extend ASM2d, the floc model would be built using the kinetics given by the International Association on Water Pollution Research and Control (IAWPRC) task group, to represent the reaction at each point within the floc. The process rate equation (see Table A4) is thus modified as shown above.

CHAPTER 4

4. CALCULATIONS AND RESULTS

4.1 Analytical solutions of non-linear equations

Initially, the process rate equations for ASM2d must be taken into consideration, to calculate the effectiveness factors ρ_F , ρ_{PP} , ρ_{PAO} and ρ_{AUT} .

It can be assumed that the steady state of oxygen distribution within the floc is:

$$\frac{\partial S_O}{\partial t} = 0$$

By applying this condition to Equation 4.15:

$$\frac{D}{R^2} \left(\sum_{k=1}^{m+2} B_{i,k} * S_{O,k} + \frac{2}{l} * \sum_{k=1}^{m+2} A_{i,k} * S_{O,k} \right) + r_i = 0 \quad 4.1$$

The factor r_i can be calculated from Equation 3.2:

$$r_i = -0.6 * \rho_4 - 0.6 * \rho_5 - 0.2 * \rho_{11} - 0.6 * \rho_{13} - 18 * \rho_{18}$$

Where:

$$\rho_4 = \mu_H \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_F}{K_F + S_F} \cdot \frac{S_F}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H$$

$$\rho_5 = \mu_H \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_A}{K_F + S_F} \cdot \frac{S_A}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H$$

$$\rho_{11} = q_{PP} \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot \frac{K_{MAX} - X_{PP}/X_{PAO}}{K_{PP} + K_{MAX} - X_{PP}/X_{PAO}} \cdot X_{PAO}$$

$$\rho_{13} = \mu_{PAO} \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot X_{PAO}$$

$$\rho_{18} = \mu_{AUT} \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_{AUT}$$

The boundary condition can be identified by the following Equations at $i = 1$ and $i = m + 2$ which are considered as the conditions at the center and the surface of floc respectively.

$$\sum_{k=1}^{m+2} A_{1,k} * S_{O,k} = 0, \quad i = 1 \quad 4.2$$

$$S_{O,m+2} = S_O^b, \quad i = m + 2 \quad 4.3$$

For the collocation points, the value of the dimension length consists of 6 collocation points (0, 0.069, 0.330, 0.670, 0.931 and 1) (Henze et al., 1987).

By applying the orthogonal collocation technique to solve the algebraic system, with Equations 5.1, 5.2 and 5.3, and using the Newton-Raphson numerical method, the result given is the radical value of oxygen along the destination radius of a single floc, in terms of 5 floc distributions with different radiuses.

4.1.1. Effectiveness factors of a single floc

The main objective of the analysis presented by these equations, and of determining the calculated dissolved oxygen concentration along the radius of the floc, is to identify factors affecting the activated sludge manner. This can be performed by taking into account the overall effect of each type of floc size separately.

Firstly, the effectiveness factors ρ_F , ρ_{PP} , ρ_{PAO} and ρ_{AUT} are described as the ratio for the rates calculated with the oxygen concentration within the floc:

$$\rho_F = \sum_{i=1}^n \frac{S_{O,i}/(K_F+S_{O,i})}{S_O^b/(K_F+S_O^b)} * \frac{\Delta V_i}{V} \quad 4.4$$

$$\rho_{PP} = \sum_{i=1}^n \frac{S_{O,i}/(K_{PP}+S_{O,i})}{S_O^b/(K_{PP}+S_O^b)} * \frac{\Delta V_i}{V} \quad 4.5$$

$$\rho_{PAO} = \sum_{i=1}^n \frac{S_{O,i}/(K_{P.o2}+S_{O,i})}{S_O^b/(K_{P.o2}+S_O^b)} * \frac{\Delta V_i}{V} \quad 4.6$$

$$\rho_{AUT} = \sum_{i=1}^n \frac{S_{O,i}/(K_{A.o2}+S_{O,i})}{S_O^b/(K_{A.o2}+S_O^b)} * \frac{\Delta V_i}{V} \quad 4.7$$

Where :

$$S_O^b = S_{O,m+2}$$

ΔV_i : the volume of i th shells and V is the whole floc.

n : total number of shells.

K_F : Saturation coefficient for growth on S_F

$K_{P.o2}$: Saturation coefficient for oxygen in part of Phosphorous accumulating organisms

$K_{A.o2}$: Saturation coefficient for oxygen in part of Autotrophic Organisms (X_{AUT})

K_{PP} : Saturation coefficient for poly-phosphate.

4.1.2. Overall effectiveness factors

The floc is widespread in the activated sludge, and occurs in different sizes. Each separate level of size has a direct impact on the rate of the reactions. Therefore, the effect of all these sizes is expressed separately.

$$(\rho_F)_{total} = \sum_{k=1}^5 w_k * \rho_F \quad 4.8$$

$$(\rho_{PP})_{total} = \sum_{k=1}^5 w_k * \rho_{PP} \quad 4.9$$

$$(\rho_{PAO})_{total} = \sum_{k=1}^5 w_k * \rho_{PAO} \quad 4.10$$

$$(\rho_{AUT})_{total} = \sum_{k=1}^5 w_k * \rho_{AUT} \quad 4.11$$

w_k : the weight of k th size of the floc

4.2 Operating conditions

To apply the orthogonal collocation method to the process equation, the matrices A and B are required, as are the boundary conditions, which depend on the dissolved oxygen concentrations in the reactor in steady state conditions.

In terms of size floc distribution, it seems to be that the information regarding the distribution of floc is not available from WWTP, therefore, the data from the literature (Zeng et al., 2005) has been used to calculate the coefficients.

Table 4.1: Distribution of flocs with different radiuses

Floc radius (μm)	32	64	128	256	512
Distribution	0.12	0.06	0.34	0.38	0.1

The value of the dispersion coefficient of oxygen within a floc can be obtained from the optimised parameters of the autotrophic and heterotrophic oxygen saturation constants in the activated sludge model ASM1 (Tyagi et al., 1996).

$$D = 1.2 \times 10^{-4}$$

The effect of the floc size and oxygen consumption is considered under working conditions, as shown in the table below:

Table 4.2: Assumed operating conditions

S_F gCODm^{-3}	S_A gCODm^{-3}	S_{NH4} gNm^{-3}	S_{PO4} gPm^{-3}	S_{SALK} mole.m^{-3}	X_H gCODm^{-3}	X_{PHA} gCODm^{-3}	X_{PAO} gCODm^{-3}	X_{PP} gPm^{-3}	X_{AUT} gNm^{-3}
30	20	8	1.8	6	780	30	45	6	53

The dissolved oxygen equation will be:

$$S_6 = 1.7 \rightarrow S_6 - 1.7 = 0$$

4.3 Results

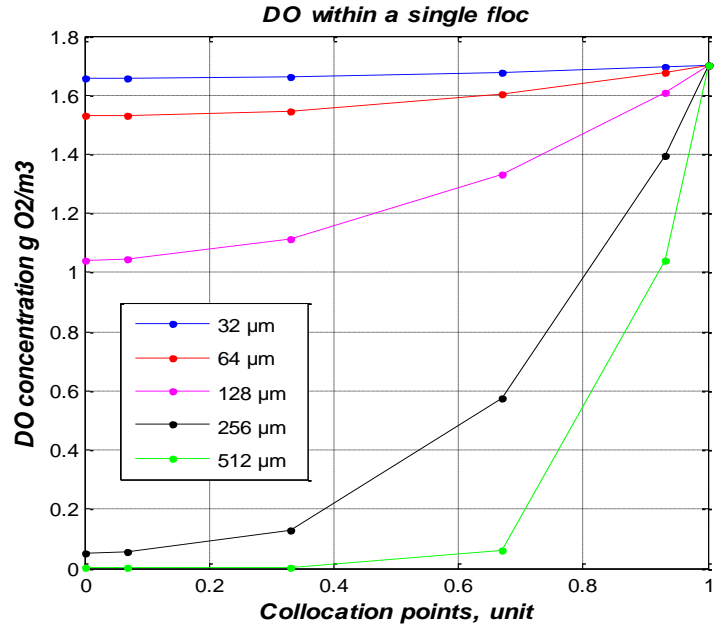
To solve the equations by Newton-Raphson, the MATLAB program was utilised to calculate the effectiveness factors. The results are shown in table 4.3.

Table 4.3: The spread of oxygen within different floc sizes

		Oxygen concentration for each shell (gO_2m^{-3})						Effectiveness factors (single floc)			
		SO_1	SO_2	SO_3	SO_4	SO_5	SO_6	ρ_F	ρ_{PP}	ρ_{PAO}	ρ_{AUT}
Floc Radiuses (μm)	32	1.6568	1.657	1.6615	1.6762	1.6942	1.7	0.802	0.725	0.53	0.35
	64	1.5285	1.5293	1.5471	1.6053	1.6769	1.7	0.802	0.725	0.53	0.35
	128	1.0415	1.0446	1.1112	1.3326	1.6098	1.7	0.807	0.806	0.79	0.71
	256	0.0507	0.0534	0.1292	0.5746	1.3971	1.7	0.806	0.79	0.72	0.52
	512	0.001	0.0015	0.003	0.0586	1.0383	1.7	0.807	0.78	0.65	0.465
Overall effectiveness factors								0.6264	0.7905	0.7392	0.703

The gradient for the dissolved oxygen concentration within the flocs varies from one size to another, as shown in Figure 4.1. A balance of components could be attained when the rate of consumption of the oxygen is almost equal to that within the floc. Balance appeared in floc sizes $32\mu m$ and $64\mu m$, in which the concentrations of dissolved oxygen within the floc were approximately the same as the oxygen ($1.7 gO_2m^{-3}$) in the bulk phase and during the aerobic phase. Denitrification took place in the large floc sizes, $256\mu m$ and $512\mu m$, which led to neither complete penetration nor the depletion of oxygen. Consequently, an anoxic zone appeared in the floc, and the aerobic reaction rate decreased.

Figure 4.1: Dissolved oxygen within a single floc



To understand the behaviour of components under nitrification and denitrification processes within a reactor, figure 4.2 presents the nitrogen components (ammonium plus ammonia nitrogen S_{NH4} and Nitrate plus nitrite nitrogen S_{NO3} and phosphate S_{PO4}). There is a sudden increase of ammonia of up to 12 gN m^{-3} during the influent load. With respect to phosphate, this has the same manner as ammonia; however, it has a different value of more or less 4 gP m^{-3} . In the aerobic period which there is no load, ammonia is converted to nitrate and nitrite (nitrification); therefore, nitrite increases.

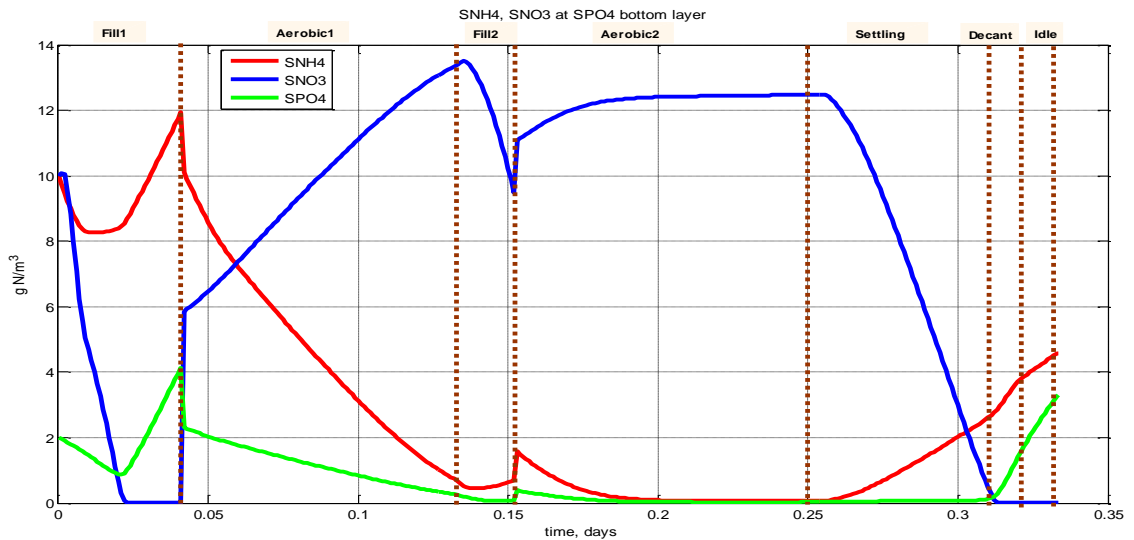


Figure 4.2: Typical cycle response during 1st period

4.4 Discussion

Sin (2007) recommended a possible extension to the ASM2d model, with respect to modelling the EBPR systems. This extended model needed to be further extended with the integration of aerobic nitrite inhibited P-uptake for further study.

Figures 4.3 and 4.4 show the N and P composition profiles for experimental data, ASM2d model and floc model at the top of the tank (water not sludge) during the sedimentation stage. There is no any addition of a carbon source for denitrification.

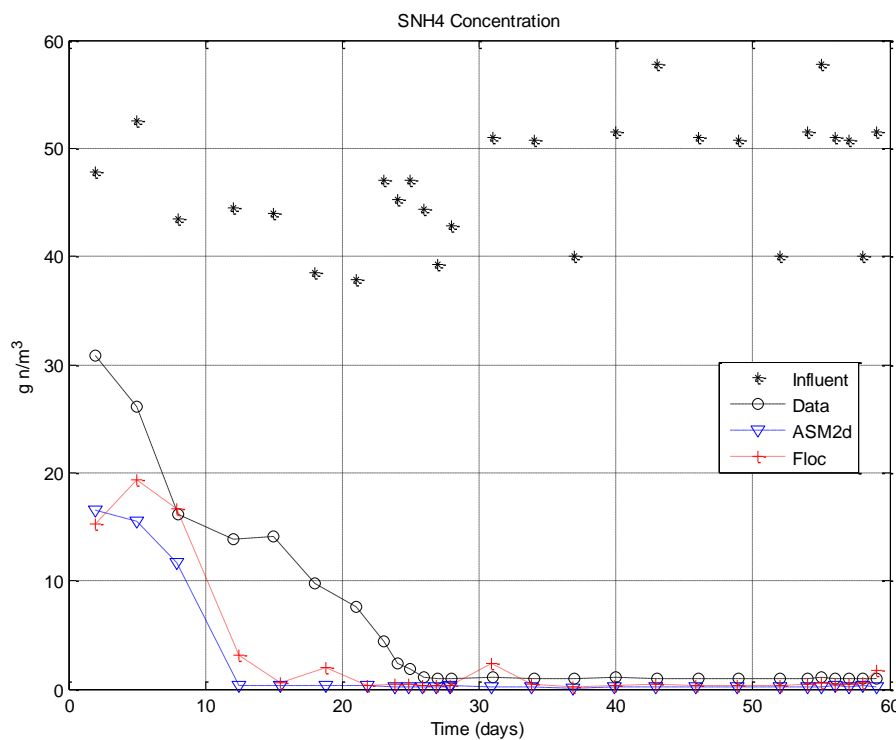


Figure 4.3:
Ammonia
concentration
 S_{NH4}

The absence of nitrate produced in the system relates to the high values of effluent and ammonia concentrations. Figure 4.3 shows that, over 20 days, the ammonia concentrations will fall. After this period, to maintain itself at a low level, the nitrate will start to rise slightly in the effluent simultaneously, as predicted from the stoichiometry of the nitrification. After 35 days, a decrease in the concentrations of effluent ammonia and nitrates was observed. However, this means that in the later stages, the nitrification process will not be performed properly.

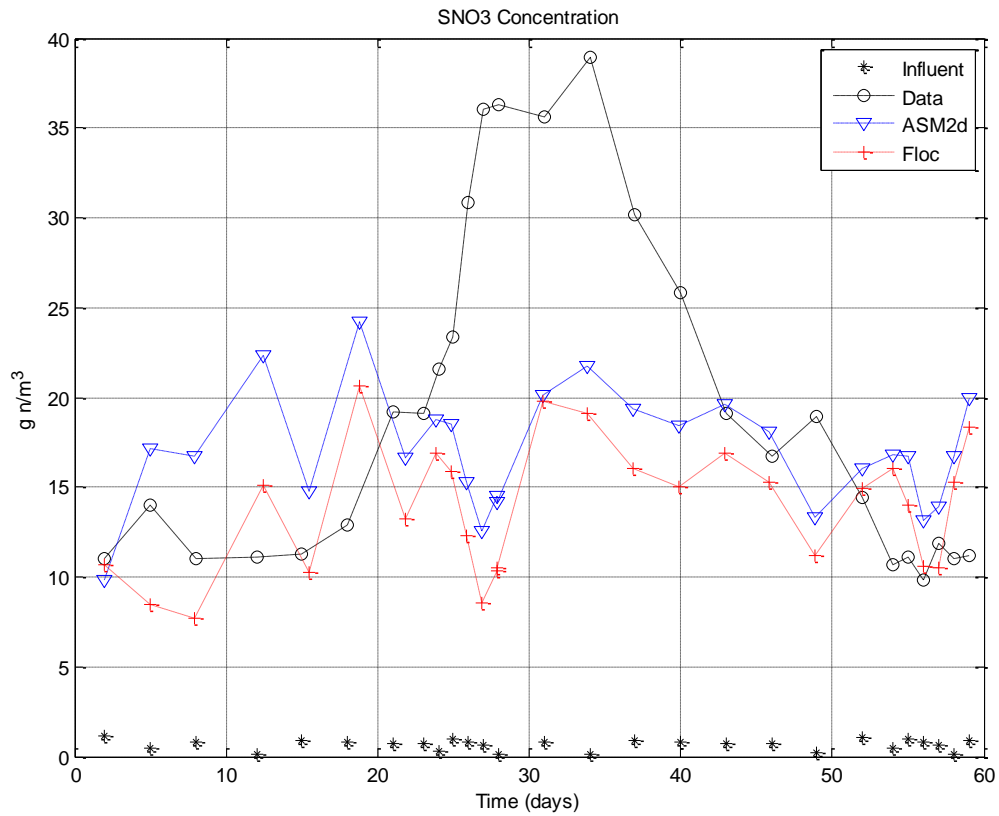


Figure 4.4: Nitrate plus nitrite nitrogen concentration (S_{NO3})

Ammonia was oxidised into nitrate and nitrite, delivering a higher concentration of S_{NO3} in comparison to the initial concentration of ammonia after 10 days. Figure 4.4 shows that, in terms of the concentration of ammonia in the experimental setup, the concentration of nitrates over 15 days (25 – 40 days) was higher. The presence of organic nitrogen, such as, amino acids and urea in the real wastewater, was the primary reason for this (Wang et al., 2006).

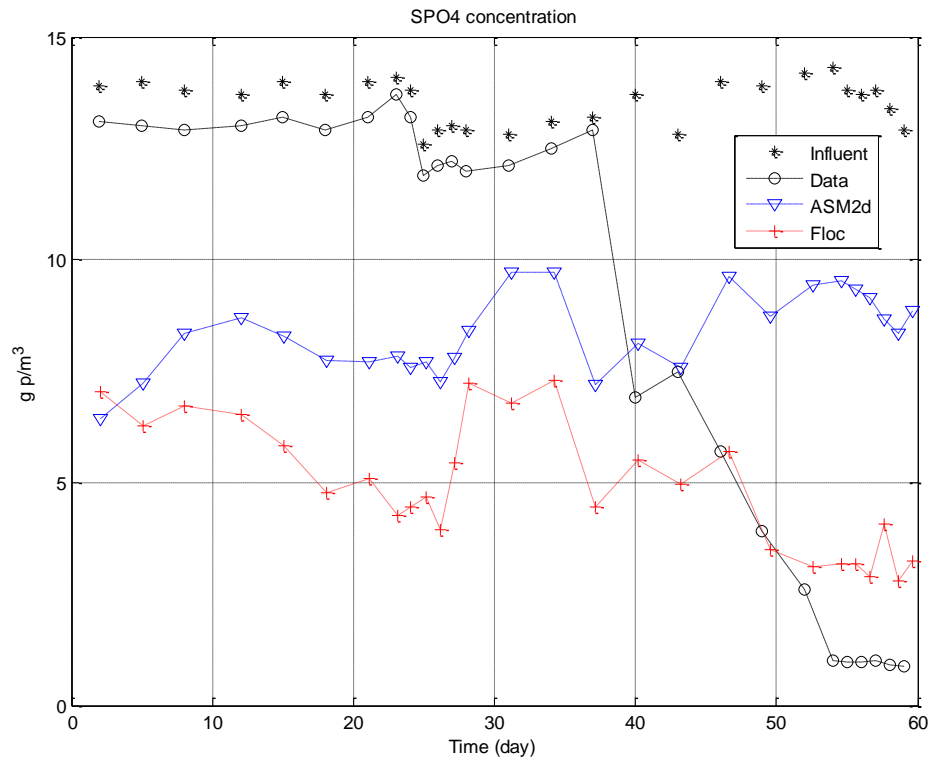


Figure 4.5: Soluble phosphorous concentrations (orthophosphates)

The rate of release of PAOs reduced in the presence of nitrate during the anaerobic phase. This is because nitrates start the process of denitrification, denitrifying ordinary heterotrophic organisms using VFA as a carbon source. PAOs can consume acetate and release phosphates at their maximum rate, only after nitrate has been completely removed from the system.

The phosphorous concentrations remaining in the reactor were maintained within 8-10 gP/m^3 and 4-7 gP/m^3 for the ASM2d model and the Floc model respectively (Figure 4.5). Moreover, fluctuations in phosphorous content were observed until the 38th day at 12-14 gP/m^3 . There was a marked improvement in the removal of phosphorous content on the following days for both the experimental and floc model. The release of phosphorous during the anaerobic step, and removal during the aerobic step were the main reasons for this. This showed that the floc factor was coming into effect.

It is possible that bacteria, using nitrate as an electron acceptor, were responsible for phosphate removal; COD was removed in the anaerobic phase in the absence of nitrate. Two observations are possible here: Firstly, the PAOs released phosphorous in the absence of electron acceptors according to the influent COD load, owing to the incomplete aeration under the increased organic loadings. In the second scenario, phosphorous may have been released due to the exhaustion of the PHA pool, due to endogenous decay metabolism. In the absence of a PHA pool for phosphorous consumption, phosphorous may be released (Lim et al., 2000).

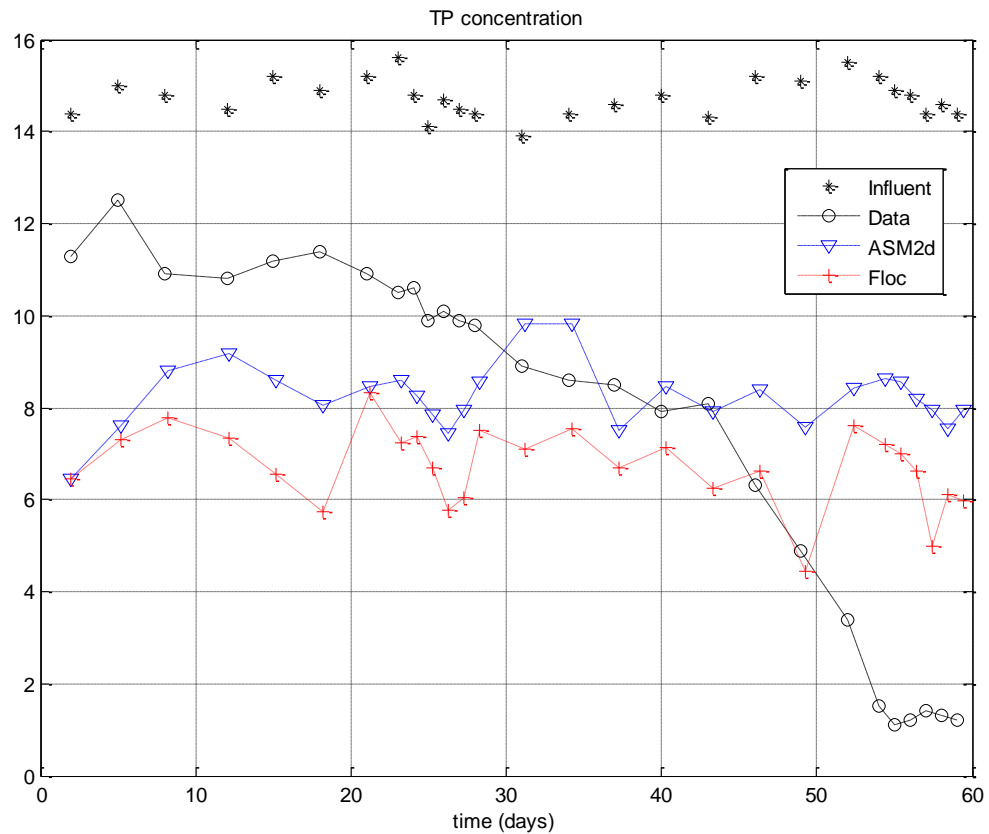


Figure 4.6: Total Phosphorous concentration TP

The total concentrations of nitrogen in both the ASM2d and floc model processes are shown in figure 4.7. These readings do not conform to the experimental data, although the ammonia and nitrate concentrations show that the two systems conform with the experiment by a large margin. As indicated in the figure 4.7, the characterisation of nitrogenous material in the influent respects the total Kjeldahl nitrogen (TKN). As stated by Dold, (2003), the division of TKN into sub-components is not especially important. Therefore, system behaviour should not be studied by assessing the standard of TN concentration individually, without considering the ammonia, nitrite and nitrate concentrations.

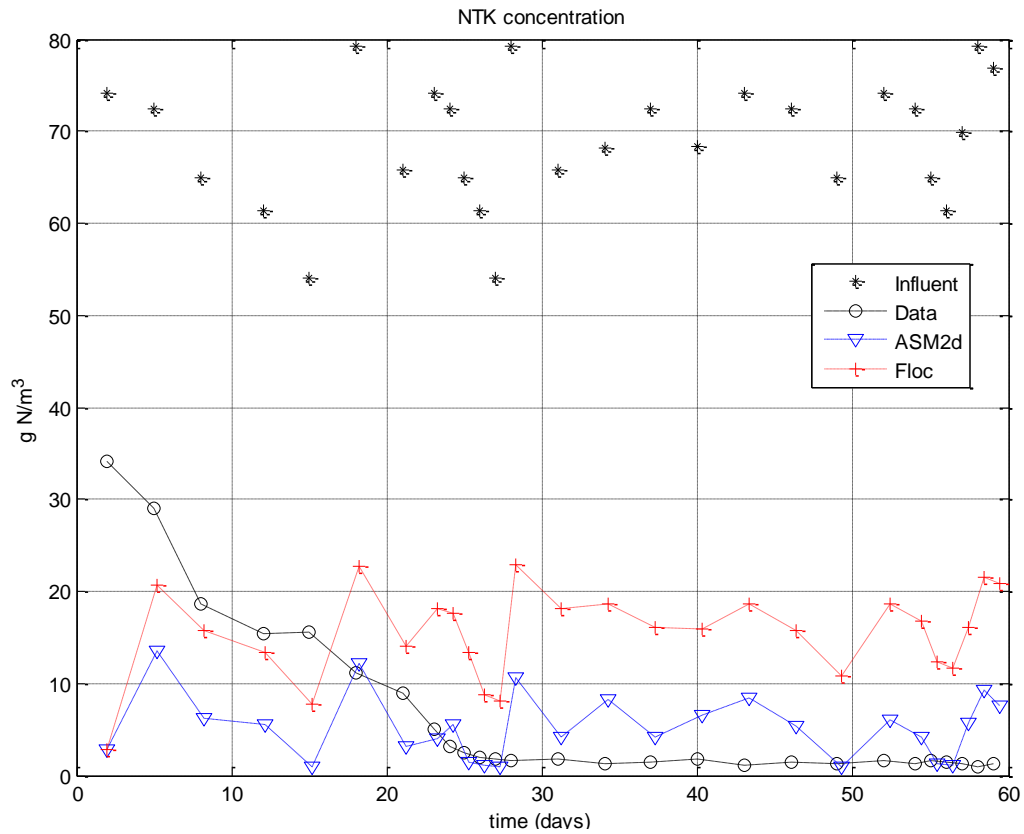


Figure 4.7: Total Kjeldahl Nitrogen concentrations TKN

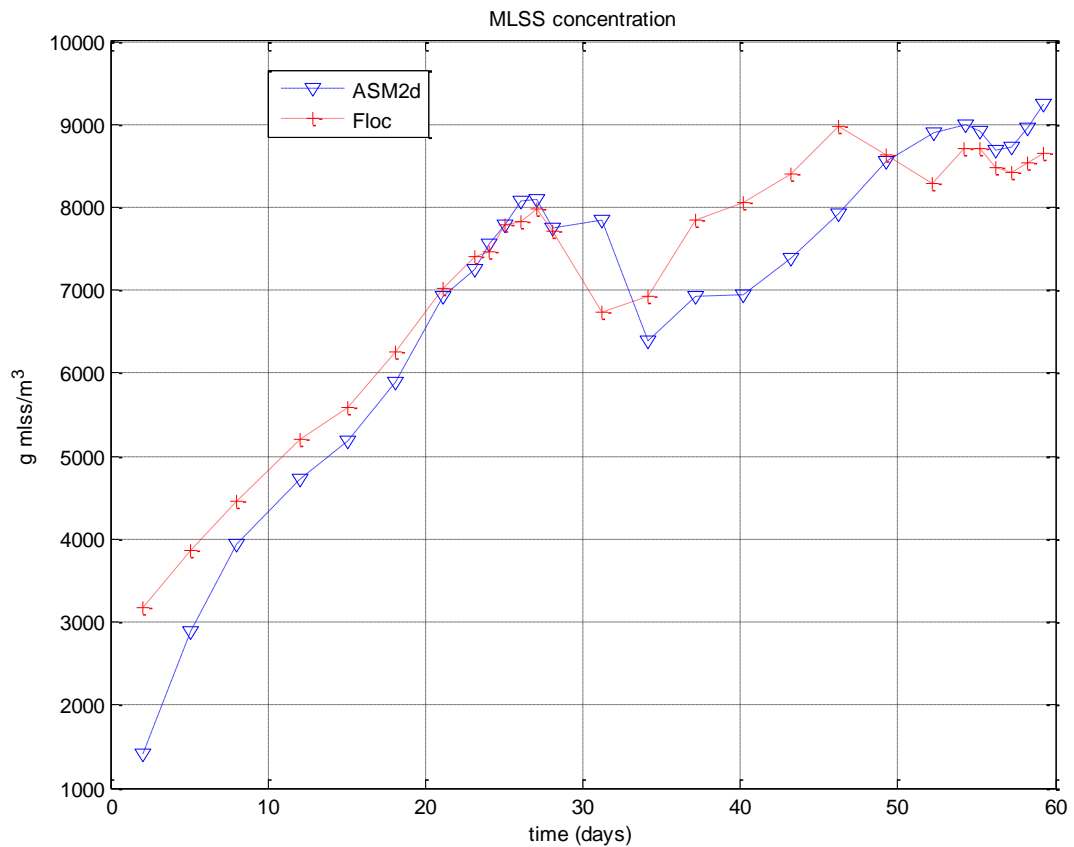


Figure 4.8: Mixed-Liquor Suspended Solids concentrations MLSS

An increase of about 50% in the MLSS is evident in the final part of the figure. From 10 days onwards, the average MLSS was around $4.5 \text{ gSS}/\text{m}^3$; this continued until the 60 day point, when the average was about $8.5 - 9 \text{ gSS}/\text{m}^3$. The rise in MLSS concentrations was due to the change in the influent feeding system. Consequently, the increase in the influent loads eventually the result. This in turn led to an increase in sludge production and an increase in MLSS concentrations, as the sludge wastage rate remained constant at this time. The presence of activated sludge systems responded to a change in the input characteristics, which led to a corresponding increase in the concentration level of MLSS (Figure 4.8).

CHAPTER 5

5. CALIBRATION PROCEDURE AND SIMULATION ANALYSIS

5.1 Calibration process

It would be problematic to adopt a strictly mathematical optimisation in the case of WWTP, because of the complexity and consequent unrecognisable nature of the significantly nonlinear stimulated sludge model. The reliance on process knowledge in a model calibration is more workable. However, significant expertise is required to establish process knowledge. In various WWTP model studies, a combination of a process engineering calibration and a mathematical approach is undertaken through the application of sensitivity analysis to verify the sensitive nature of the model to changes in parameters that are modified when conducting the calibration procedure (Insel et al., 2003).

Since complex search and optimisation problems are characterised with intricate interactions and nonlinearities, there are numerous optimal solutions available; however, the majority have inferior objective function values. With the aim of finding solutions to this problem, traditional methods often focus only on locally optimal solutions. The calibration process could be done using computer-based automatic techniques, such as genetic algorithms, using an overall objective function.

5.2 Genetic Algorithm Approach

A GA is based on evolution and the process of natural selection, in which emphasis is placed on survival of the fittest. The GA has developed into an influential search and optimisation technique to solve problems involving objective functions that are neither differentiable nor continuous. Recently, GA-based approaches have been successfully utilised to optimise complicated bioprocesses (Petersen, 2000).

Initially, a population of parameters is necessary when applying a GA. Each of the parameters have an initial population group. In this section, the initial values of the parameters will be default values given in the ASM2d model. There is a need for a fitness evaluation function. This would calculate the combined responses of parameter values, as well as generate their respective fitness value. The expression of a general fitness function would be as follows:

$$F = \sum_{i=1}^n |x_i - v_i| \quad 5.1$$

Where: n number of samples (data size), x is the model output and v is the reference data.

The above fitness evaluation functions would provide the summation for errors arising between the reference (experimental data), as well as the output of the simulation model for the various set of parameters utilising the SIMULINK program by using objective function which consists of four measurable variables ammonia, nitrate, nitrite and phosphors concentrations. The purpose here is to minimise the fitness function F using the Genetic Algorithm.

5.3 Floc model calibration

There is an undoubtedly direct relationship between the parameter estimation quality and the practical identifiability of parameters, which impinges on the ability to use available experimental data to acquire accurate parameter estimates. In this section, the effectiveness floc factor will be calibrated with remain the rest of parameters as it is in ASM2d benchmark model.

5.3.1 Parameters Estimation

The floc model provides a standardised set of basis activated sludge models, with nominal parameter values and effectiveness floc parameters, as suggested in the previous chapter. Nonetheless, some adjustments were made to some of the model parameters to ensure good predictive capability.

Since no method has the ability to provide values in a precise and accurate way, it is imperative to perform tests in order to establish the most appropriate values. However performing tests requires a lot of effort, especially if the tests are very complex. Rangel-Merino (2005) states that genetic algorithms can produce remarkable results when searching for optimal values from high dimensional and non-linear functions.

In terms of parameters estimation using GA, all parameters are subjected to the fitness evaluation function, with the functions obtaining initial responses for every solution. Responses can then be used to calculate the fitness value of the fitness function as aforementioned. Notably, the aim when undertaking the GA involves minimising the fitness value.

5.3.2 Floc calibration results

The specifications for the study are as follows: the size of the population is 30, the number of variables in the fitness function is 4, and the generation size is 80. Moreover, the fitness function will be a multi-objective function, which combines ammonia and soluble phosphor objective functions. The calibration process, as carried out over the first 20 days and the next 40 days, is used to validate the model by applying correlation criteria.

- GA results

Figure 6.1 displays the best fitness for each generation. When finding a solution, there is significant progress when lowering the fitness value. It can be seen that the best solution was found after 50 generations. Therefore, the estimated parameters will be from this generation.

Figure 5.1: Fitness value of GA versus the generation number for the floc model calibration

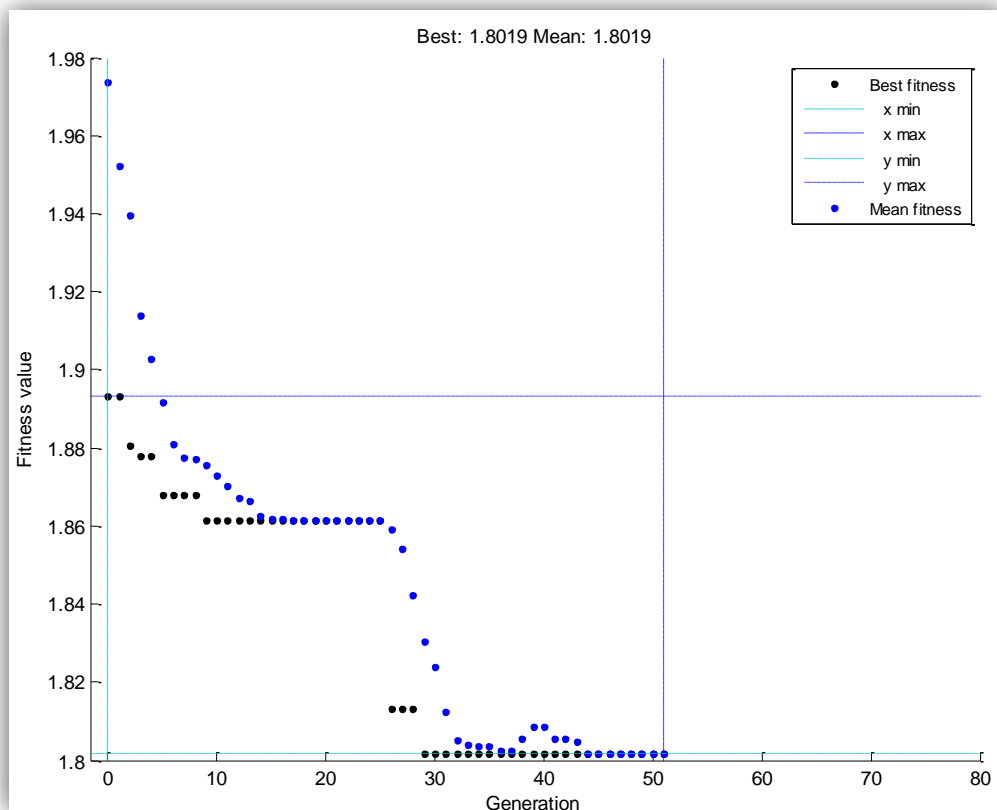


Table 5.1: Calibration results for effectiveness floc factors

Effectiveness factors	ρ_F	ρ_{PP}	ρ_{PAO}	ρ_{AUT}
Numerical calculations	0.62	0.79	0.74	0.703
GA estimation	0.45	0.68	0.71	0.7

- **Correlation results**

Ammonia levels can be reduced using a sequencing batch reactor during the aeration-mixing phase. At this stage, the ammonium nitrogen was transformed into oxidised nitrogen, and nitrification subsequently allowed to release ammonia into the liquid phase (Wang and Wan, 2009).

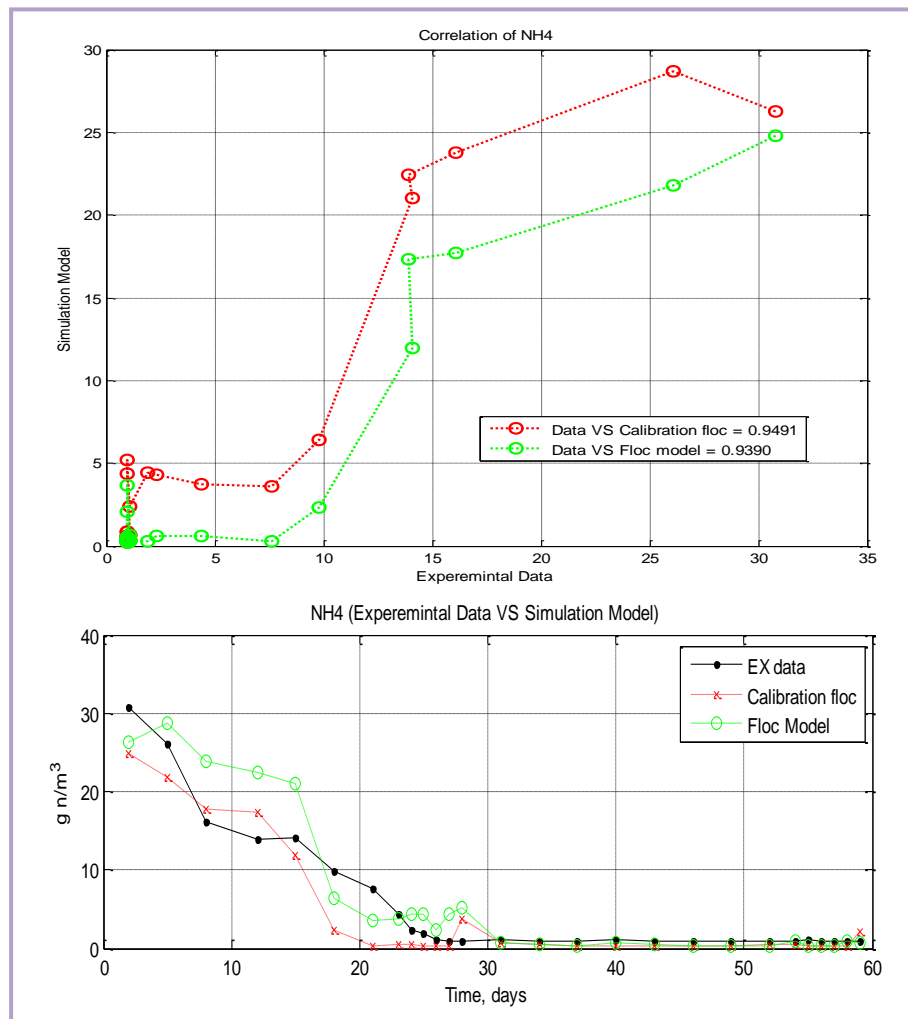


Figure 5.2: Correlation coefficient and ammonia concentration curve of (floc factors calibration).

As shown in Figure 5.2, the amount of ammonia, including the liquid phases for both the effectiveness floc, and calibration model, was similar to that in the experiment, and both models have a better correlation. The correlation of the calibration is slightly less than in the floc model due to the phosphate uptake and additional heterotrophic activity, which consumed the majority of the oxygen during the aerated phase.

Figure 5.3 illustrates that both the nitrate in the calibration model and the modified floc model were in the range of $10 - 20 \text{ gO}_2\text{m}^{-3}$, with a reasonable correlation of 0.66 and 0.69 respectively. However, the decrease in nitrates was offset by an improvement in the amount of phosphorous removal.

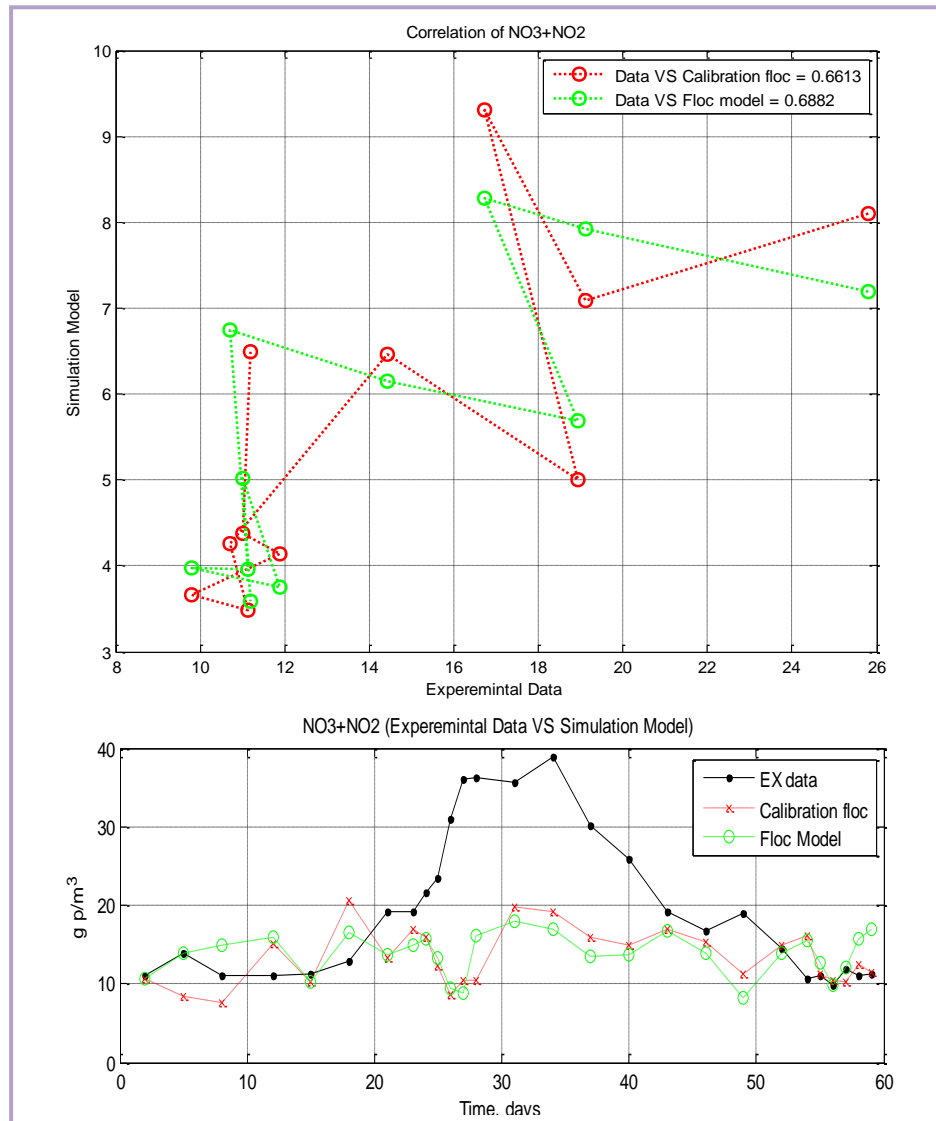


Figure 5.3: Correlation and concentration curve of nitrate plus nitrite nitrogen (floc factors calibration).

In the process of PAOs; phosphate S_{PO4} can be released from polyphosphate X_{PP} under anaerobic conditions. Nevertheless, the PAOs must gain energy from the aerobic conditions to enable orthophosphate S_{PO4} storage, in the form of internal cell polyphosphates X_{PP} (Jung et al., 2004).

Figure 5.4 demonstrates that the correlation coefficient between the experimental and model values were 0.85 for the calibration model, but the floc model attained a value of 0.76.

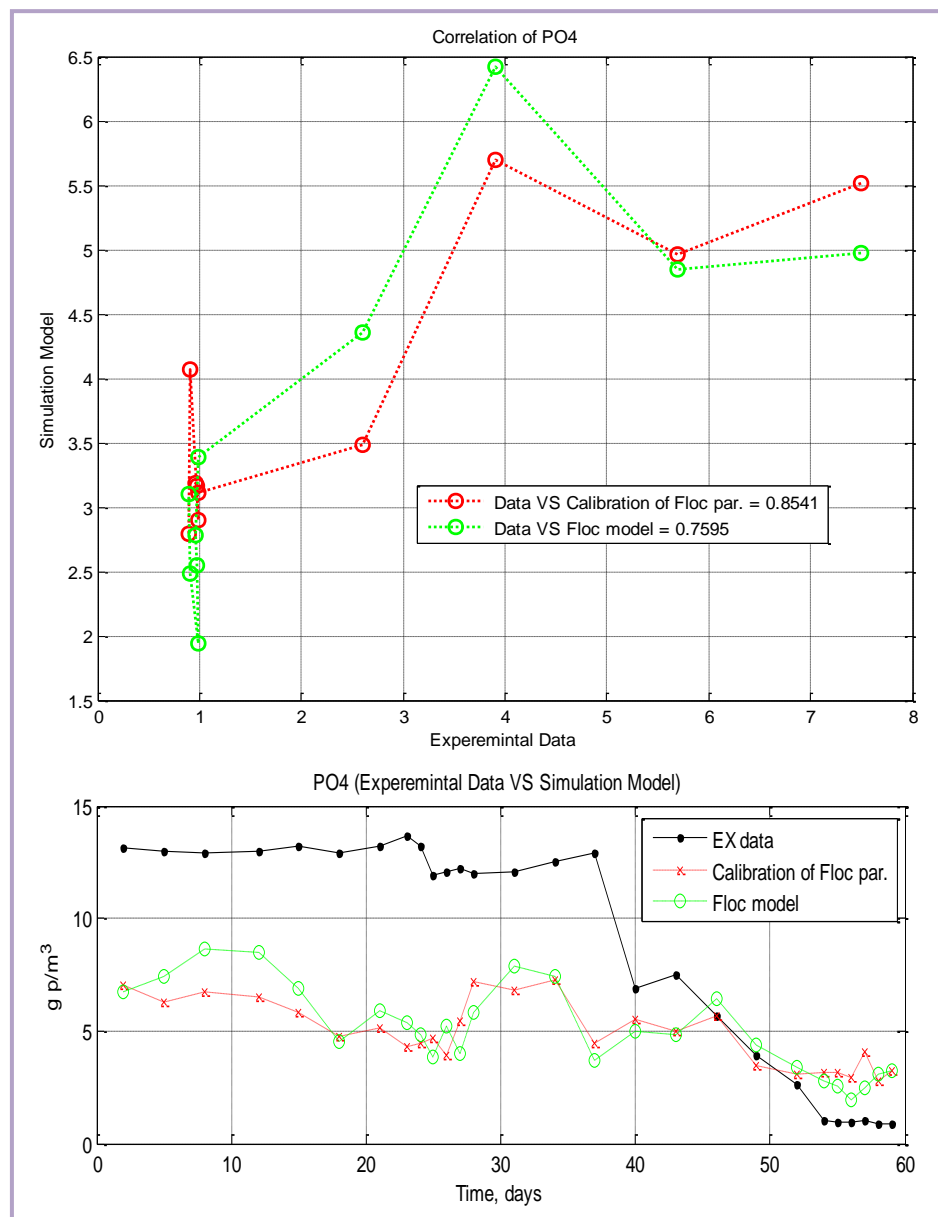


Figure 5.4: Correlation and concentration curve of phosphorus (floc factors calibration).

5.4 Calibration of ASM2d parameters

In line with IAWQ ASM2, the default parameters that Henze et al. (1995) provided were adopted when initialising the SBR model. The simulation results were slightly different from the experimental results observed with respect to the NO₃-N and PO₄-P concentrations in the effluent.

Although, only heterotrophs possess denitrification ability in the ASM2 model, Furumai's (1999) focus was mainly on denitrification observable in phosphorous accumulating organisms (PAOs).

When extending the Activated Sludge model ASM2d, there is a need to calibrate the main stoichiometric coefficients and kinetic constants. In line with Serralta (2004), gradual changes were made to the values of the model's kinetic parameters, with the aim of minimising the sum total of the squared relative deviations resulting from the concentration profiles that arise from simulation and from measurements.

In the current work, expert knowledge was combined with process knowledge. This approach is common to the selection of parameters to fit various models to data, such as in IWA guidelines (Henze et al., 2000). Therefore, the range (maximum and minimum) of the parameters in table 5.2 was obtained from the literature (Rieger et al., 2013, Henze et al., 1999, Dudley et al., 2002).

A number of stoichiometric and kinetic parameters for phosphorous accumulating organisms (PAOs) were included to calibrate the model.

Table 5.2: Values of stoichiometric and kinetic parameters

Parameters	Definitions	Units	ASM2d default	Min	Max
Typical stoichiometric parameters					
Y_{PO4}	PP requirement per PHA stored	$gP/gCOD$	0.4	0.26	0.64
Y_{PAO}	Yield coefficient (biomass /PHA)	$gCOD/gCOD$	0.625	0.58	0.9
Phosphorous accumulating organisms (PAOs)					
q_{PHA}	Rate constant of PHA storage	d^{-1}	3.0	0.36	9.03
μ_{PAO}	Growth rate of PAO	d^{-1}	1.0	0.67	2.97
$b_{PAO},$ $b_{PP},$ b_{PHA}	Lysis rate of $X_{PAO}, X_{PP},$ X_{PHA}	d^{-1}	0.2	0.04	0.27
K_{PS}	Saturation coefficient for phosphorous in storage of PP	mgP/m^3	0.2	0.2	0.5

5.4.1 ASM2d calibration and validation

In terms of the GA specifications for ASM2d calibration, the size of the population is 40, the number of variables in the fitness function is 8 (parameters calibrated) and the generation size will be 80. Moreover, the fitness function will involve ammonia and soluble phosphor objective functions. The calibration process will be carried out first over 20 days, and then for the next 40 days to validate the model by applying correlation criteria as well as comparing between literature values.

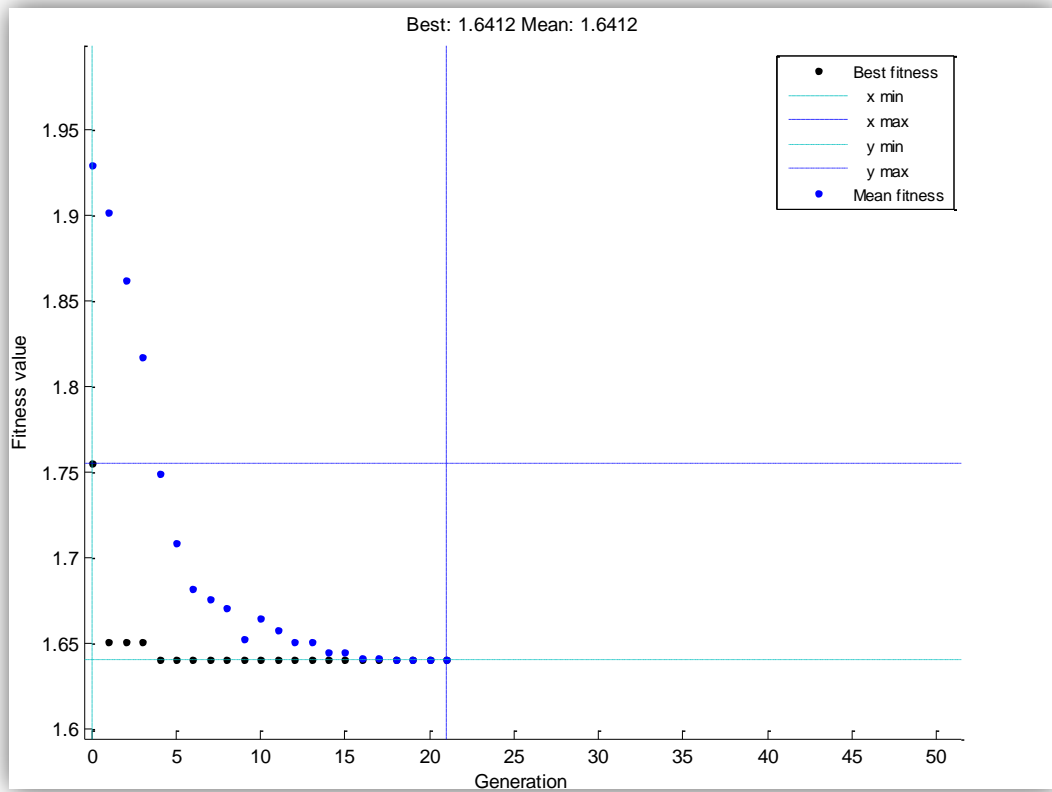


Figure 5.5: Fitness value of GA versus generation number for ASM2d model calibration

The best solution was found after the 21st generation (Figure 5.5); thus, the parameters will be estimated at this generation.

If the same values are used for the parameters, it is not necessary to reproduce the experimental results, as this will not be acceptable. In comparison to the default values proposed in the ASM2d ($Y_{PO4} = 0.4$), the Y_{PO4} obtained are higher, although not significantly higher than those proposed by the other authors. However, the authors attained similar values from the various experiments in which they utilised an SBR.

Phosphorous concentrations could be managed by Y_{PAO} and Y_{PO4} , more so than the bio kinetic parameters, according to the study by Soejima et al. (2008).

The yield coefficient in the case of Poly-P is necessary; in every PHA stored, Y_{PO4} was increased to $0.62 Y_{PO4}$.

Table 5.3: ASM2d calibration results

Parameters	Definitions	Units	ASM2d default	SBR calibration
Y_{PO4}	PP requirement per PHA stored	$gP/gCOD$	0.4	0.62
Y_{PAO}	Yield coefficient (biomass /PHA)	$gCOD/gCOD$	0.625	0.76
q_{PHA}	Rate constant of PHA storage	d^{-1}	3.0	2.8
μ_{PAO}	Growth rate of PAO	d^{-1}	1.0	1.57
$b_{PAO},$ $b_{PP},$ b_{PHA}	Lysis rate of X_{PAO}, X_{PP}, X_{PHA}	d^{-1}	0.2	0.25
K_{PS}	Saturation coefficient of PP	mgP/m^3	0.2	0.23

The slow degradation of biodegradable COD is a critical issue, when simulating active sludge systems, because it is responsible for ensuring genuine profiles of electron acceptors that are dependent on space and time. For the purpose of simplification, increments were only limited to a yield of PHA coefficient, which rose to 0.76 from 0.625. In this case, this could increase the availability of the carbon source to be denitrified simultaneously with EBPR, through the maintenance of lower levels of dissolved oxygen (Barker and Dold, 1997). However, some reports indicate that the configuration, Y_{PAO} , and the rate, significantly influence noncommittal phosphorous release, the PAO, X_{PP} and the discharged phosphate concentrations contained in the bulk liquid (Insel et al., 2003, Govoreanu et al., 2003).

A rise in the growth rate of PAO from 1.0 to 1.57 was carried out with the aim of raising PAOs activity under conditions of limited oxygen.

In the case of PHA, the maximum storage rate q_{PHA} was calibrated to $2.8gCOD/gcellCOD.d$, which was close to the 3.0 that Henze et al. (1999) suggested. Studies undertaken by Çinar et al. (1998), on steady state calibration in the case of oxidation, implied EBPR could only be achieved if the q_{PHA} were set to $8.0g COD/gCODd$, using the ASM2 model. Otherwise, it would not be possible for X_{PAO} to compete with regular heterotrophs, because they lack the capacity to build up a PHA pool to facilitate biomass growth, and storage of Poly-P. In addition, the q_{PHA} values provided in the literature vary from 3.0 to $8.0 gCOD/gCODd$ (Ekama and Wentzel, 1999a, Çinar et al., 1998, Wentzel et al., 1990).

The lysis rates for X_{PHA} , X_{PP} and X_{PAO} were calibrated at $0.25d^{-1}$. Any adjustment in the lysis rates for the X_{PHA} , X_{PP} and X_{PAO} parameters could facilitate moderate constancy in the bioreactor's PAO concentrations. Consequently, PAOs can utilise PHA efficiently. Comparable calibration results and observations were found for values $0.14d^{-1}$, as Çinar et al. (1998) suggested. The hypothesis suggested from this is that the PAOs lower their endogenous metabolism so they can compete with the remainder of the heterotrophs in conditions where there are low nitrate/oxygen concentrations (Brun et al., 2002).

Finally, adjustments and improvements in the parameters render the predictions of effluent quality more accurate, as provided in Table 6.3. The remaining parameters are similar to those mentioned regarding ASM2d. However, after the parameters for those simulations were adjusted, a reasonable difference was observed when comparing effluent containing nitrate and nitrite, ammonia and phosphors, with the experimental data provided.

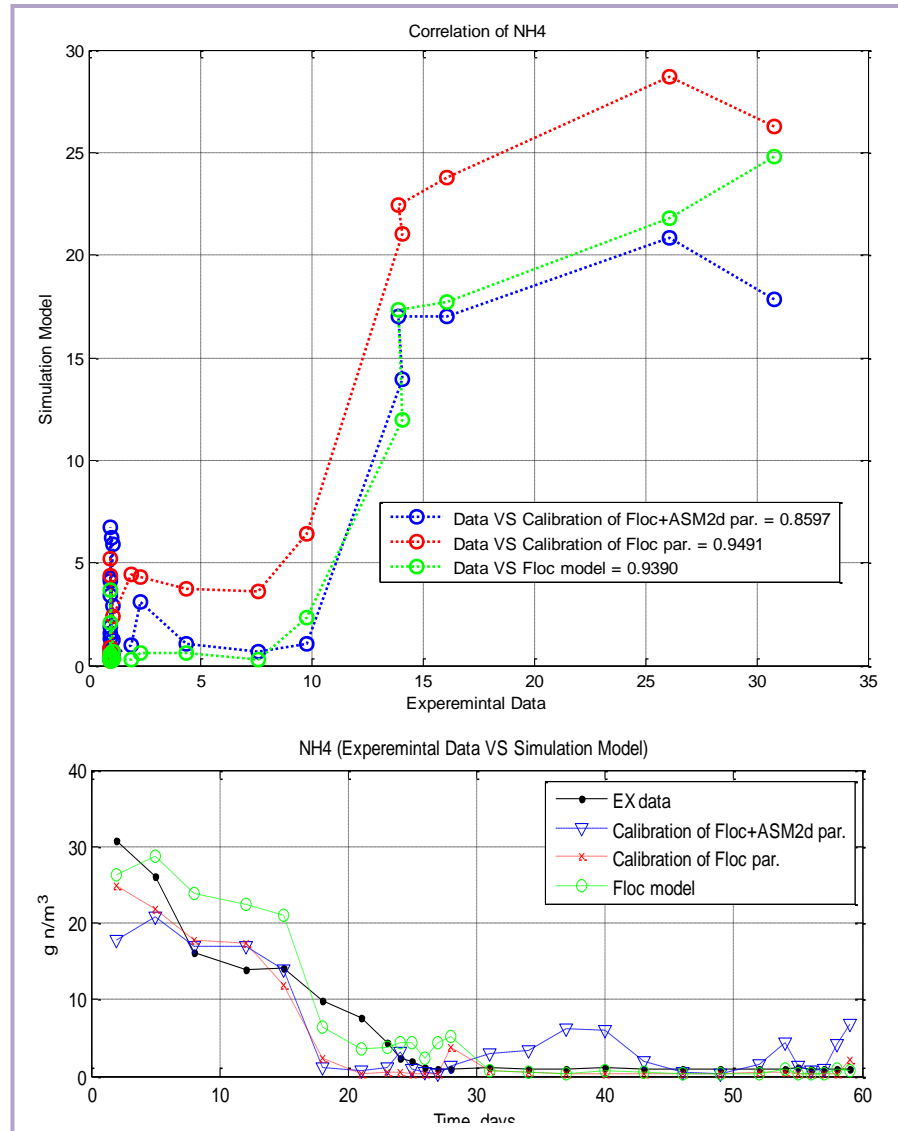


Figure 5.6: Correlation coefficient and ammonia concentration curve (ASM2d model calibration).

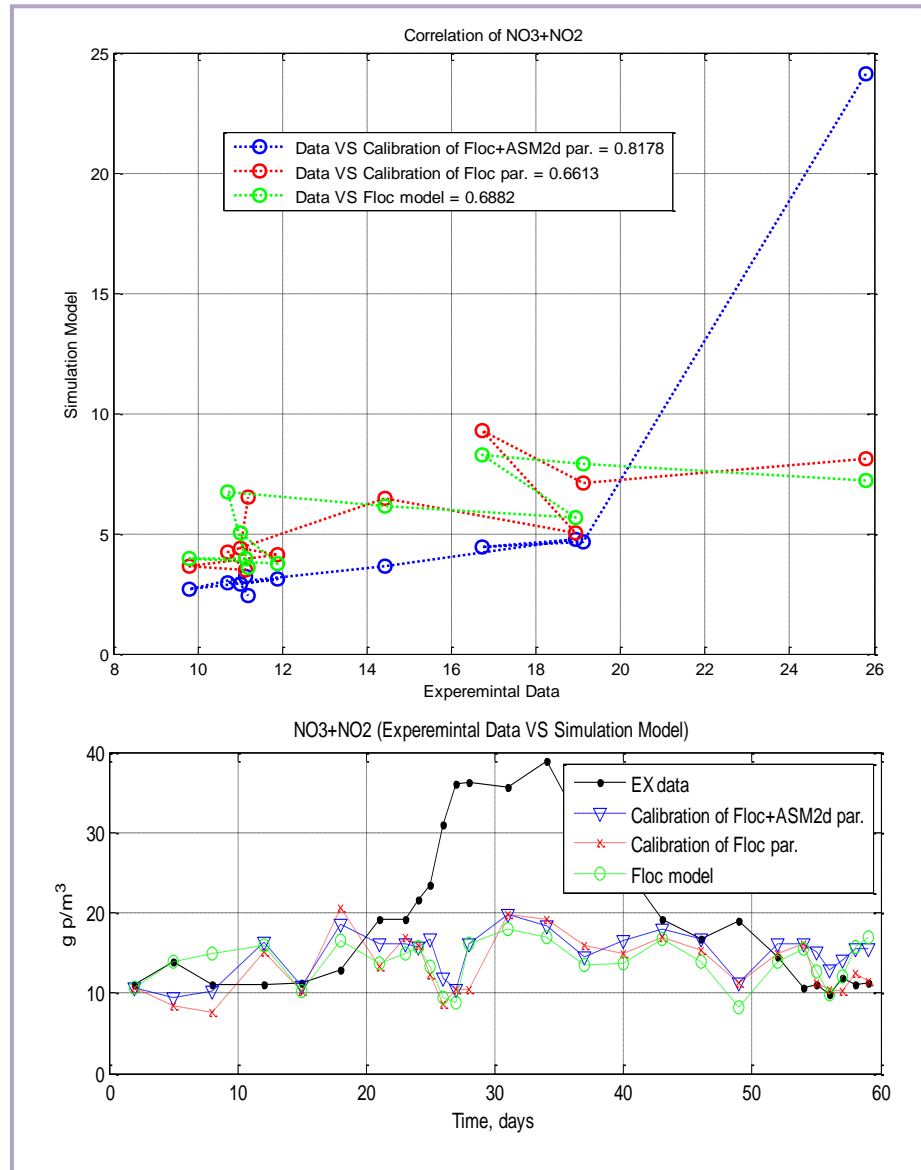


Figure 5.8: Correlation and concentration curve of nitrate plus nitrite nitrogen (ASM2d model calibration).

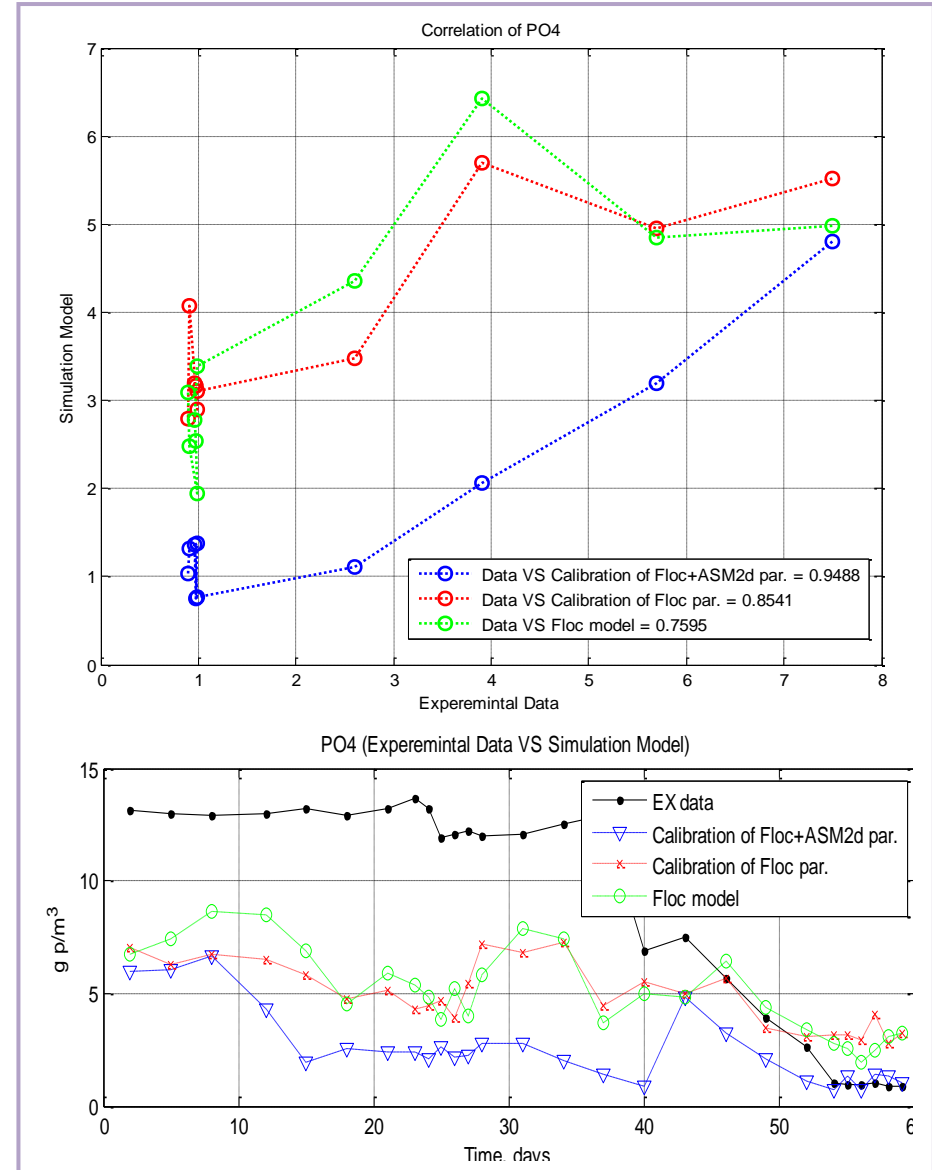


Figure 5.7: Correlation coefficient and phosphorus concentration curve (ASM2d model calibration).

CHAPTER 6

6. SLUDGE ACCESS OPTIMISATION

6.1 Introduction

The process could be optimised by controlling the SRT, especially during the activated sludge process, which tends to be essential to facilitate wastewater treatment. The SRT determines the rate of growth of microorganisms in the activated sludge process.

In addition, controlling the SRT permits a simple and real-time calculation to adjust the wasting flow rates, with the aim of maintaining a target SRT and stability in a microbial population. In situations where there is no control, or where the control is poor, the mixed liquor constitutes a group of microorganisms not optimised for the prevailing growth conditions.

Biological phosphorous removal (BPR) from wastewater tends to be achieved by using PAOs to enrich activated sludge. It is possible for PAOs to accumulate phosphorous in bacterial cells that are stored as polyphosphate (polyp) granules when excess levels are normally necessary to satisfy the demands for metabolic growth. The storage process is ordinarily known as enhanced BPR (EBPR). Over the decades, numerous treatment plants have been designed and developed with the aim of reducing both organic nitrogen carbon and phosphorous through the EBPR process.

The consequences of the removal of activated waste sludge have the potential to produce a high percentage efficiency range for phosphorous removal. Despite some disputes regarding the precise bacterial composition of these microorganism communities, they are generally acknowledged as PAOs.

Sources of volatile fatty acids (VFAs) are created by the fermentation of organic matter in the anaerobic zone, especially propionate and acetate, which also successively serve as sources of foods for PAOs. Notably, PAOs are anaerobic bacteria, even though they are not capable of reproducing in an anaerobic environment. They exhibit a unique capacity to consume VFAs when subject to strict anaerobic conditions and consequently store intracellular carbon compounds. PAOs obtain energy for the process through the metabolism of stored polyphosphate reserves. This results in phosphorous being released during the specific phase.

During the aerobic phase of the process, PAOs can multiply and absorb phosphate that will then replace the supplies exhausted during the anaerobic phase. Through the oxidation of the carbon reserves accumulated in the anaerobic phase, PAOs have the capacity to increase stored phosphate, especially under aerobic conditions, in comparison with that released during the anaerobic phase, since the stored energy produced through the aerobic oxidation of the carbon compounds exceeds the energy consumed when storing them during anaerobic phases. However, accumulation of nitrates is likely to hinder the development of the BPR process, despite the fact that during the aerobic phase, ammonia is converted into gaseous nitrogen products concurrent with P uptake.

6.2 Solids retention time (SRT)

The SRT is the time that microorganisms spend in the system. It can also be interpreted as the period available in which microorganisms can reproduce, and the sludge age. Every organism has its own regeneration time, which is dependent on numerous factors. In the event that the SRT exceeds the regeneration time for a specific organism, that organism proliferates. If the reverse is the case, the organism will be washed from the system.

6.3 SBR control

Sludge recirculation, dissolved oxygen (DO) and sludge wasting are operating parameters that are controllable in different circumstances. The DO concentration is controlled in the aerobic zone with the simulation. Whereas, SRT depends on MLSS in the aerobic zone. Sludge wasting normally happens after the settlement stage, due to the MLSS having been reached to assure a maximum concentration of solids. This wastage can take place every cycle, which is daily or even weekly

Currently, automation of the DO control has generated immense debate, due to the amount of energy required to integrate automation. Nevertheless, SRT that is controlled via sludge wasting emerges as the most crucial parameter of the design and operation in terms of influencing the performance, as exhibited by the activated sludge systems (Boontian, 2012).

In the SBR reactor, the resulting value when dividing the mass of solids during the aeration stage by the mass of the wasted solids (no any sludge return) represents the sludge retention time SRT. Solid mass could be determined by multiplying tank volume

by mixed liquor concentration TSS under aerobic. Also, wastage of solid mass could be determined by multiplying the flow of wasted sludge with the mixed liquor concentration TSS of the wasted sludge.

$$SRT(day) = \frac{\text{Mass of solids in Reactor (gTSS)}}{\text{Mass of wasted solids } (\frac{gTSS}{day})} \quad 6.1$$

It is possible to control the SRT, in the case of granular sludge SBR, through daily sludge discharge. For instance, for a 10-day SRT to be maintained, a tenth of the reactor sludge ought to be discharged daily. Notably, a short SRT tends to favour the development of PAOs. Whereas, maintenance of an SRT exceeding 10 days ought to be done to facilitate complete nitrification (Tchobanoglous et al., 2003).

6.4 Impact of SRT

Generally, a higher SRT is associated with greater biodiversity. Whereas, the risk of an SRT that is too low lies in that it might not support particular functions. This is especially critical in the case of nitrification, as it is the only pragmatic mechanism for removing ammonia. Additionally, denitrification would not occur if there were no nitrification. Whereas, a SRT that is too high would raise the operating costs while reducing the system's treatment capacity. Achievement of optimum settling would depend on the prevalence and diversity of microorganisms. In the case of SRT that is too low, organisms would predominate, while pin floc would occur in cases where SRT is too high.

Hu et al. (2003) observed the effect of varying aerobic mass fractions (and consequently anoxic mass fractions) and short sludge ages on system performance as regards N- and P-removal.

6.5 Results and discussion

In this section, the impact of access time on the biological removal of phosphorous and nitrogen will be examined, taking into account the time required to access the sludge, which indicates that sludge access will be achieved every cycle, i.e. every day and every two days.

With regard to evaluation, nutrient removal is evaluated in terms of the percentage at which efficiency is attained. This efficiency regularised the data in relation to the influent concentration.

Tables 6.1 and 6.2 present the percentage efficiency of ammonia and phosphor removal at different SRTs, in reference to a number of sludge access stages.

Table 6.1: Ammonia removal efficiency

<i>Sludge taken</i>	Every cycle			Every day			Every 2 days		
	1-20	21-40	41-60	1-20	21-40	41-60	1-20	21-40	41-60
<i>EX Data</i>	60.01	94.82	98.00	60.01	94.82	98.00	60.01	94.82	98.00
<i>SRT 11d</i>	59.32	92.57	90.89	83.36	77.17	74.28	85.25	85.87	89.27
<i>SRT 9d</i>	61.77	92.54	96.34	72.56	99.10	97.93	73.59	87.16	83.36
<i>SRT 7d</i>	46.41	72.62	93.76	65.68	86.61	98.05	70.46	64.63	87.63
<i>SRT 5d</i>	24.74	2.04	-2.89	68.26	86.84	40.78	69.69	59.17	44.57

Table 6.2: Phosphors removal efficiency

<i>Sludge taken</i>	Every cycle			Every day			Every 2 days		
	1-20	21-40	41-60	1-20	21-40	41-60	1-20	21-40	41-60
<i>EX Data</i>	6.01	5.01	78.38	6.01	5.01	78.38	6.01	5.01	78.38
<i>SRT 11d</i>	52.01	52.13	42.60	56.14	60.92	64.80	51.00	71.25	34.52
<i>SRT 9d</i>	35.04	37.64	42.60	33.43	45.09	49.69	52.95	47.41	34.52
<i>SRT 7d</i>	40.75	68.54	66.07	70.77	78.30	66.13	70.56	75.52	39.62
<i>SRT 5d</i>	30.17	9.29	51.34	69.12	81.30	90.98	54.43	69.26	72.14

6.5.1 Sludge access every cycle

In the case of Figures 6.1 and 6.2, a comparison of nutrient removal was conducted for different wastewater plants, and the average percentage of ammonia removal (in the hydrogen form) was found to stand at 90.98, 96.34 and 93.76 percent for SRT 11 days, 9 days and 7 days respectively. During the first 20 days it stood at 59.32, 61.77 and 46.41 percent. These percentages illustrate that SRT affected the N removal.

On the other hand, when SRT is low (5days) the ammonia conversion process to nitrogen is absent and does not take place during the treatment. This is because the time is not sufficient for the growth of the bacteria which led to an increase in ammonia concentrations. When it comes to the anaerobic and aerobic phosphorous removal process, the release of phosphate S_{PO4} took place in the anaerobic phase. The process of phosphate S_{PO4} release and uptake is a strong determinant of removal efficiency. The percentage in Figure 6.1 shows that concentrations of P-effluent differed for various SRTs.

The SRTs resulted in phosphorous removal efficiencies in the range of 40.75, 68.54 and 66.07 percent during the first, second and final 20 days at SRT=7d. This indicated that there was an improvement in terms of phosphorous removal. Whereas, there was a slight decrease in efficiencies at SRT=9d.

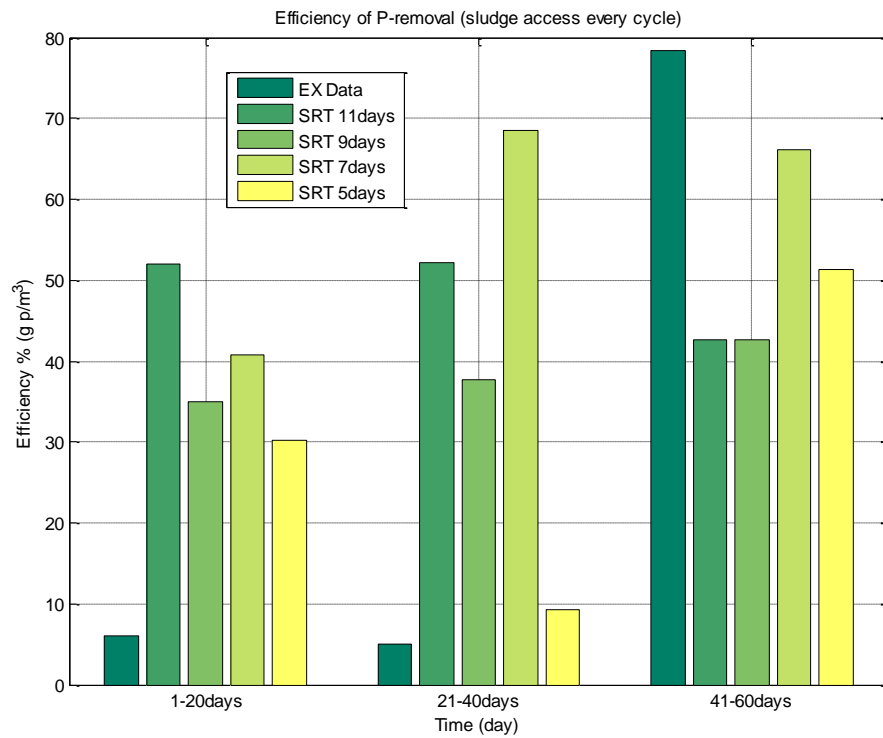


Figure 6.1: Efficiency of phosphors removal (sludge wasted every cycle)

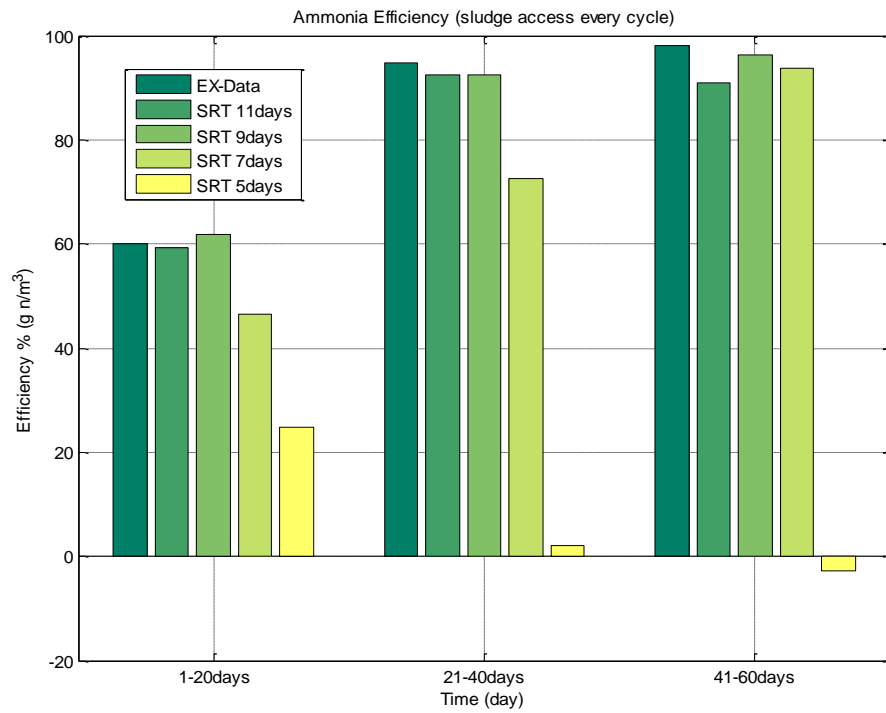


Figure 6.2: Efficiency of ammonia removal (sludge wasted every cycle)

Figure 6.3 illustrates the MLSS in instances where there were different sludge levels. It can be noted that the MLSS is low (about 2000 mg TSS/m^3) at SRT=5d, because the amount of sludge wasted was high. However, the MLSS is ($4000 - 6500 \text{ mg TSS/m}^3$) when the volume of sludge access decreased, as a result of SRT being in the range 7-11d.

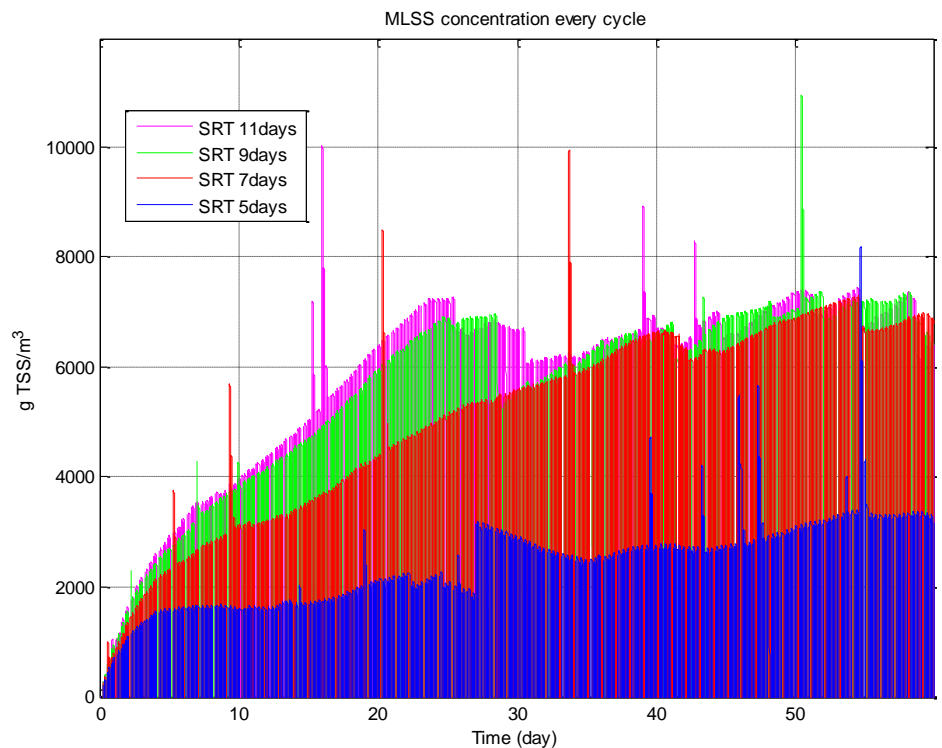


Figure 6.3: MLSS concentration (sludge wasted every cycle)

6.5.2 Sludge access every day

Figure 6.4 exhibits an increase in phosphate removal efficiency between day 10 and day 60, resulting in 33.43 and 56.14 percent removal in the initial 20 days, 45.09 and 60.92 percent in the following 20 days, while 49.69 and 64.8 percent removal took place in the final 20 days when increasing SRT from 9d to 11d. These phosphate uptakes and the polyphosphate storage are likely to result from PAOs. These results could be caused by the fact that the phosphate is released only in completely anaerobic conditions, while the uptake of phosphate in bulk liquid only occurs in aerobic conditions. Also, the MLSS is about $5000 \text{ mg TSS}/\text{m}^3$ when the volume of sludge access decreased, as a result of SRT being in the range 7-9d.

As evident in figure 6.4, the efficiency of phosphorous removal stood at 90.98 percent, and the SRT was 5d. However, the efficiency of nitrogen removal fell to 40.78 percent from 86.84 percent for the same amount of sludge access (Figure 6.5).

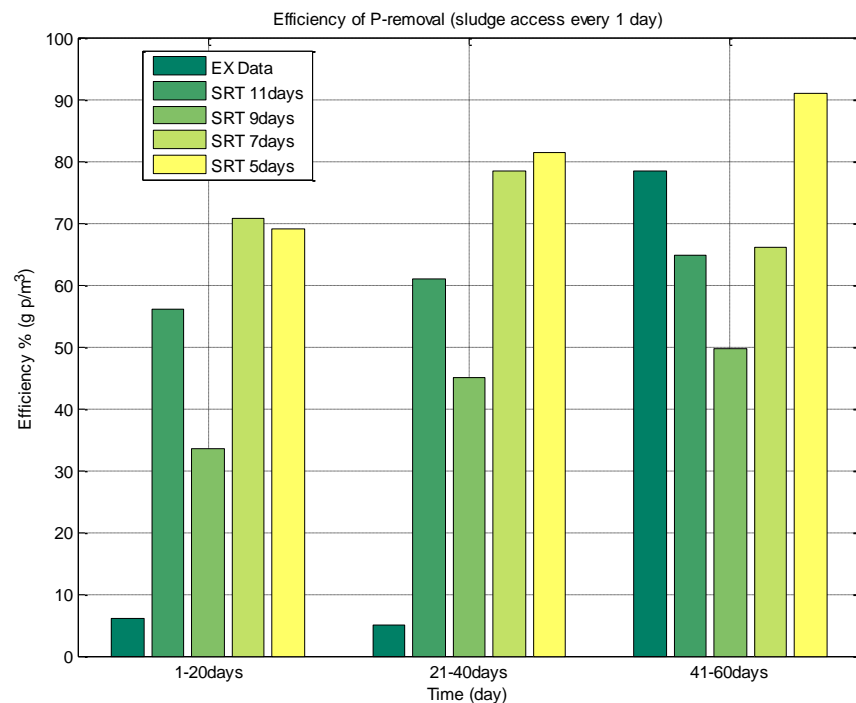


Figure 6.4: Efficiency of phosphors removal (sludge wasted every day)

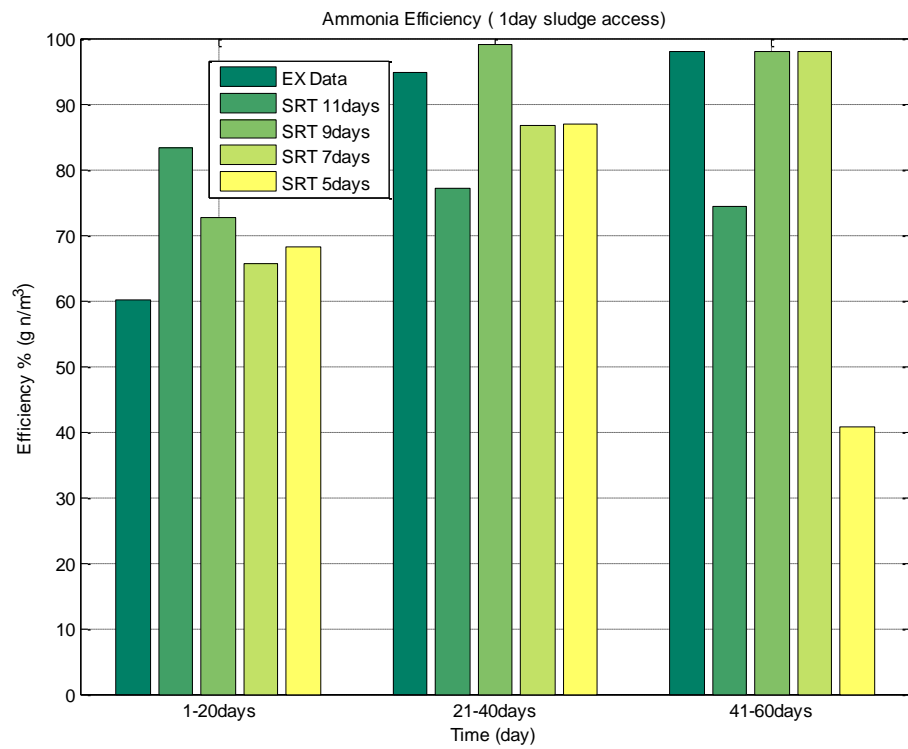


Figure 6.5: Efficiency of ammonia removal (sludge wasted every day)

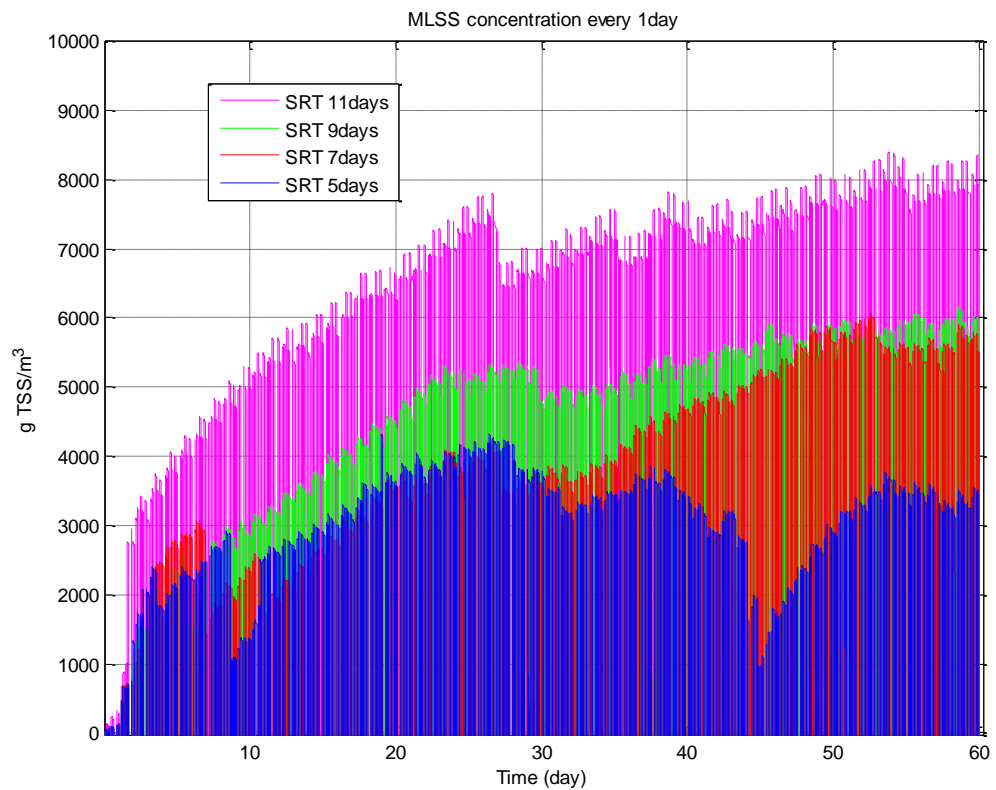


Figure 6.6: MLSS concentration (sludge wasted every cycle)

6.5.3 Sludge access every 2 days

In the case of Figure 6.7, SBR is shown to exhibit a low P-removal performance as it decreased as SRT increased (7-11d). However, ammonia concentration efficiency showed a low $\text{NH}_4\text{-N}$ removal performance as it was recorded, decreasing from 69.69 to 44.75 percent at (SRT=5d). It was suggested that the exhibition of such low removal efficiencies, as in the case of $\text{NH}_4\text{-N}$, could be attributed to the length of sludge access being inadequate to accommodate nitrifiers' growth (Li and Wu, 2014). Consequently, withdrawing the same volume of sludge as that wasted every 2 days would be inappropriate, unless it has been subjected to SRT control. This is likely to be difficult. Nonetheless, the alternative is that there is likelihood that there will be a small amount remaining at the end of the various cycles, raising the amount withdrawn at the end of each day.

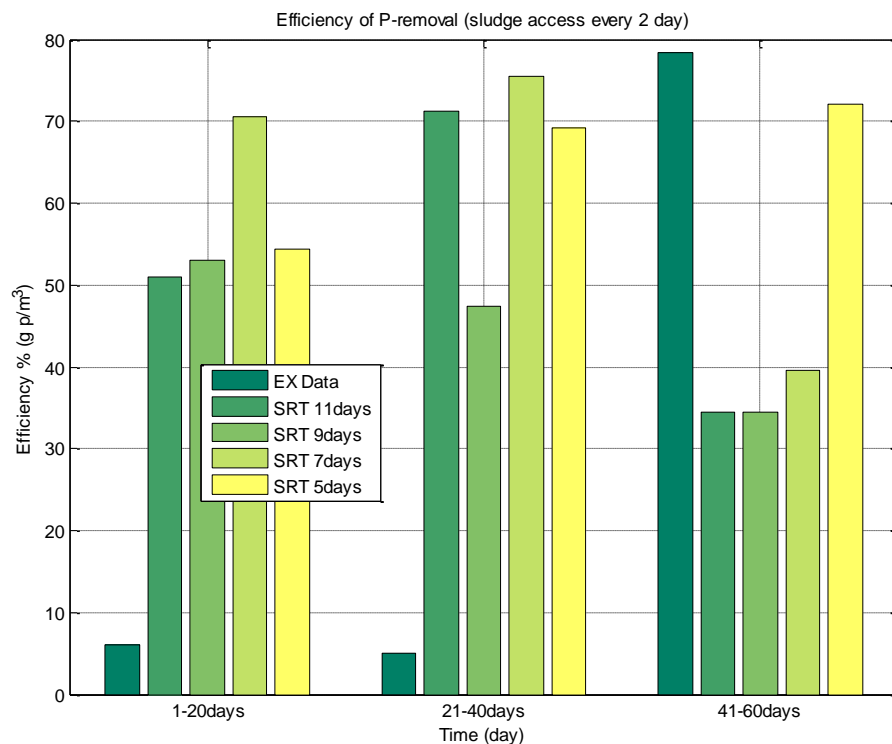


Figure 6.7: Efficiency of phosphors removal (sludge wasted every day)

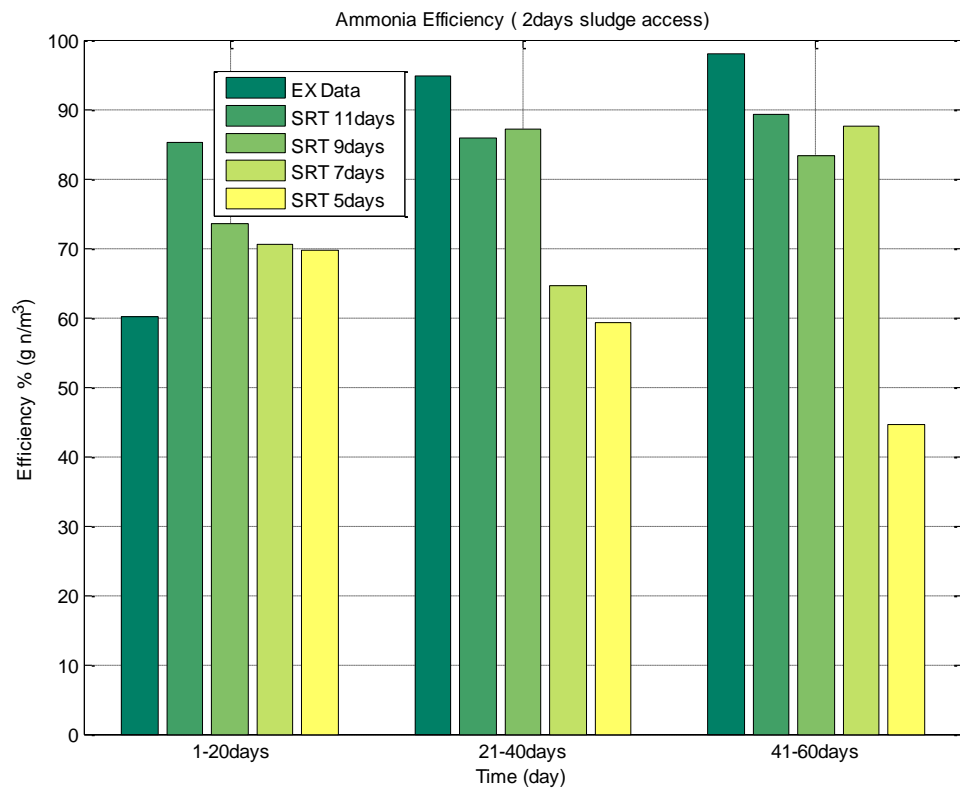


Figure 6.8: Efficiency of ammonia removal (sludge wasted every day)

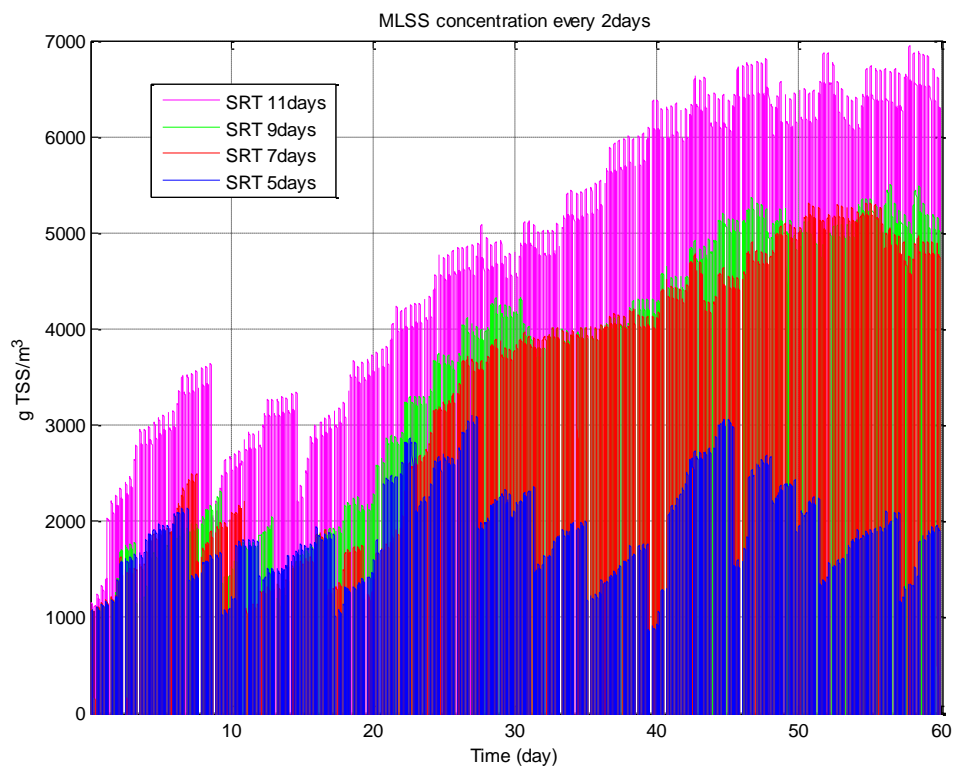


Figure 6.9: MLSS concentration (sludge wasted every cycle)

Figures 6.4, 6.5, 6.7 and 6.8 show that it can be deduced that wasting the sludge amount in a 1 day case was beneficial, as it raised the efficiency of P removal compared to the case of 2 days.

In order to obtain a phosphorous-rich biomass from the biofilm system, back-washing of filters must take place when the level of internal stored phosphorous in the bacteria is elevated. Limited net phosphorous removal is achieved due to limited sludge wasting; frequent wasting may disrupt system performance (Li and Wu, 2014).

The role that SRT plays in the determination of the dewatering characteristics of activated sludge was examined at different levels of activated sludge access. It was found that SRT plays a crucial role in determining the sludge dewatering rates. According to Pitman (1975), the dewatering rates are ideal when the SRT exceeds 11 days.

SRT can be taken as less than 11 days in the case of more reliable and effective systems. It can be concluded that simulations where SRT is between 7 and 9 days are the only ones meeting the requirement for sludge access each cycle; however, the system was slightly flexible when sludge was taken at the end of the day.

In Li and Wu's (2014) investigation, the growth of nitrifiers was controlled at a short SRT and nitrite existed in the SBR effluent. There was an increase in SS concentrations relative to increasing SRTs, while there was a decrease in excess sludge production with increasing endogenous decay with high SRTs. The minimum effluent concentration of soluble microbial products SMP was obtained at an SRT of 5 d. The nitrous oxide N₂O emission was accelerated significantly by the heterotrophic conversion of nitrate to nitrogen gas, with low DO concentrations and high oxidised nitrogen concentrations.

CHAPTER 7

7. CONCLUSION AND FUTURE WORK

7.1 Conclusion and Summary

The kinetics associated with this unique modified ASM2d model have the potential to be used to describe the lowered uptake of phosphorous and the PAOs denitrification that are experienced in practice. Thus, this unique model provides invaluable information regarding PAO kinetics when subjected to different conditions.

It can be hypothesised that the cause of the contradiction arising between the experimental and theoretical results included the mass transfer limitation applied to oxygen in the granules. Moreover, DO concentration inside the floc was found to be much lower than in its external part, and thus growth of floc is found to limit the DO inside the floc. Therefore, the limitations imposed on oxygen are that only a portion of nitrifiers can contribute to oxidising nitrogen.

In the SBR system, the sludge process has the right concentration levels of activated sludge, and is crucial to facilitate efficient nutrient removal. Therefore, this study considered the waste sludge amount, to examine its effect on the activated sludge treatment.

7.2 Summary of outputs and achievements

The main questions that were posed in this research work were:

- How can the ASM2d model be extended by creating effectiveness floc coefficients, and by examining the dynamic behaviour of this modified ASM2d model when considering the floc size distribution?
- How possible is it to develop an automatic innovative technique that can be used in the calibration of this modified ASM2d model with floc parameters to facilitate determination of whether the resultant model has the potential to achieve specific performance requirements?
- Can the significance of the floc effects on system dynamics be evaluated? Are the results of the simulations and experimental data of similar order?
- How can the optimisation of the activated sludge process be achieved by controlling the SRT and the amount of sludge access?

Based upon the outcomes of this original research work, the following points can be made regarding the posited research questions:

- Achieving optimal phosphorous and nitrogen removal from nutrient-rich industrial wastewater biological is possible, using activated sludge, operated under alternating anaerobic and aerobic conditions. The floc factors are likely to play a role in facilitating the nitrification, the denitrification, and the phosphorous removal processes as observed.

- In the calibration stage, the correlation criterion were used to compare between simulation results, calibration outcomes and the data provided. The percentile efficiency removal charts exhibited the manner in which varying the SRT impacts on plant performance. Moreover, improving the modified model's correlation with experimental results can be achieved by considering the floc effectiveness factors. After calibration of the floc parameters in the modified ASM2d model, the results were found to be in good agreement with theoretical and experimental data.
- The comparative behaviours of the biological phosphorous removal between the default benchmark model ASM2d and this unique modified ASM2d with floc model addition using the SBR reactor data revealed the results of floc model are in stronger agreement with the experimental data than the default ASM2d model.
- A long SRT would be necessary to maintain a specific level of nitrifiers while ensuring that the nitrification would be effective. Nevertheless, a long SRT has been associated with increased phosphorous removal efficiency, because of the low rate of sludge wastage, and the likelihood of phosphorous being released in the reactor.
- The results reveal that phosphorous removal efficiency decreased with the rising SRT, because of the reduced rate of biomass yield. Whereas, phosphorous removal efficiency could increase under a longer SRT, because the decay in PAOs was lower than the decay for the remainder of the microorganisms.

7.3 Future follow-on work

- Essentially, SRT is an important factor in activated sludge optimisation. Selection of SRT is accompanied with numerous consequences associated with sludge production and process performance. The conventional mechanism of SRT control could involve the manual adjustment of the sludge-wasting rate, based on the concentration of the MLSS. However, taking MLSS measurements and analysing the manual sample for MLSS should be undertaken experimentally, to calculate the sludge volume wasted for SRT control.
- The activated sludge ASM2d model has different non-linear equations, which complicate the system. Therefore, this needs to be reduced according to several mathematical components, depending on the relationship between the biomass and effectiveness parameters, which have no effect on system behaviour. This model reduction aims to apply identification in the process of N and P removal, and, therefore, to design appropriate controls for the whole system.
- For better predictions of this unique modified model, the experimental model should be rebuilt in practice, and more measurements taken, as they are appropriate for the process control. For example, the effect of sludge retention time SRT on the removal of phosphorous should be considered and accurate readings for the MLSS concentrations taken.

- In terms of control, over the past forty years, conventional controllers have been used for industrial processes. Although many of the control algorithms have been improved, it is still appropriate to control the system through modelling; largely because it can provide adequate performance to oversee most control problems. One of the most widespread methods used in the field of modern control is the model predictive control (MPC).

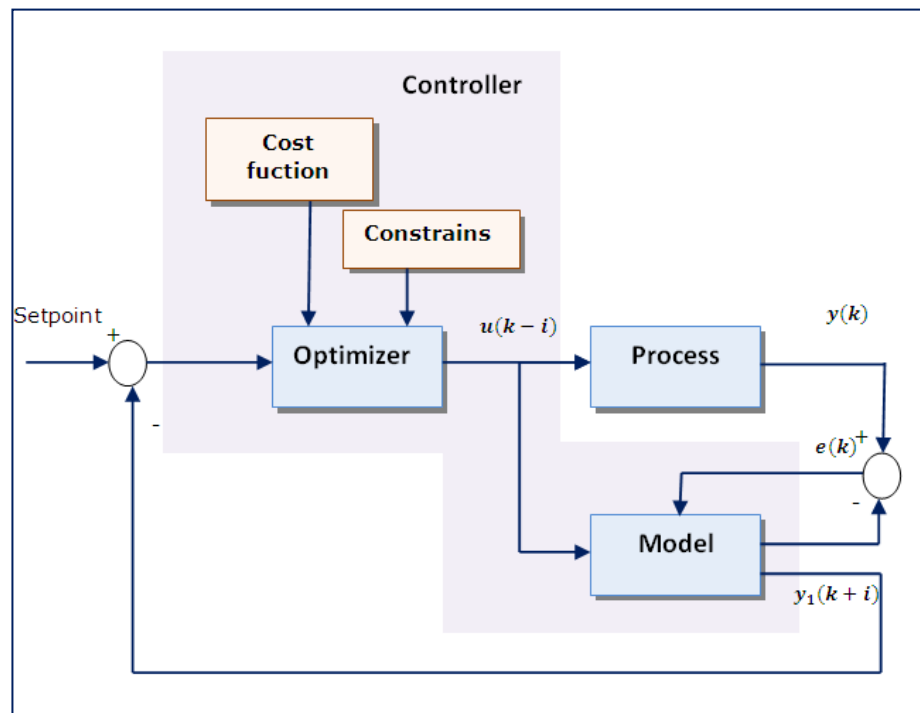


Figure 7.1: The MPC block diagram

Figure 8.1 shows the block diagram for the model predictive control MPC; it describes the installation model, integrating a process to predict and find a new model that causes a prediction error $e(k)$ between the measurement of plant $y(k)$ and the prediction model $y_1(k+i)$, which is almost zero (Eng et al, 2006). In future work, one of the applications of MPC, will mean that a non-linear model of predictive control (NMPC), will be recommended as the essential point for control system design to maintain the effluent concentration within specified limits.

- One of the problems encountered regarding to optimisation procedure is that the design and operation of biological systems should not be based on SRT values exceeding the need for the overall treatment of organic N and P removal. As a result, SRT needs to be a manipulating parameter, when it comes to the optimisation of the biological process. As a consequence, further works will consider soluble retention time factors, which qualifies as the most critical design and control parameter that the engineer has access to, as MPC parameters and the inclusion of more measurements and monitor the model performance under different conditions. Moreover, it would be desirable for future research to focus on the remaining parameters, such as bioreactor volume and oxygen concentration.

Appendix

A =

-21.0000	23.6305	-3.6799	1.8126	-1.7631	1.0000
-8.7783	6.6640	2.8405	-1.2325	1.1613	-0.6550
2.4953	-5.1848	0.7688	2.9413	-2.2496	1.2291
-1.2291	2.2496	-2.9413	-0.7688	5.1848	-2.4953
0.6550	-1.1613	1.2325	-2.8405	-6.6640	8.7783
-1.0000	1.7631	-1.8126	3.6799	-23.6305	21.0000

B =

220.0000	-311.7984	132.2532	-70.7166	70.2618	-40.0000
135.8638	-183.0297	59.6594	-20.5306	18.1743	-10.1371
-11.2855	31.8224	-36.9703	21.8257	-10.9511	5.5587
5.5587	-10.9511	21.8257	-36.9703	31.8224	-11.2855
-10.1371	18.1743	-20.5306	59.6594	-183.0297	135.8638
-40.0000	70.2618	-70.7166	132.2532	-311.7984	220.0000

Table 01: Conversation factors of ASM2d

Index c: Index i	Components	COD $i_{COD,i}$	N $i_{N,i}$	P $i_{P,i}$	Charge $i_{charge,i}$	Mass $i_{TSS,i}$
1	S_{O2}	-1	0	0	0	0
2	S_F	1	i_{N,S_F}	i_{P,S_F}	0	0
3	S_A	1	0	0	-1/64	0
4	S_I	0	1	0	1/14	0
5	S_{NH4}	-64/14	1	0	-1/14	0
6	S_{NO3}	0	0	1	-1.5/31	0
7	S_{PO4}	1	i_{N,S_I}	i_{P,S_I}	0	0
8	S_{ALK}	0	0	0	-1	0
9	S_{N2}	-24/14	1	0	0	0
10	X_I	1	i_{N,X_I}	i_{P,X_I}	0	i_{TSS,X_I}
11	X_S	1	i_{N,X_S}	i_{P,X_S}	0	i_{TSS,X_S}
12	X_H	1	$i_{N,BM}$	$i_{P,BM}$	0	$i_{TSS,BM}$
13	X_{PAO}	1	$i_{N,BM}$	$i_{P,BM}$	0	$i_{TSS,BM}$
14	X_{PP}	0	0	1	-1/31	3.23
15	X_{PHA}	1	0	0	0	0.60
161	X_A	1	$i_{N,BM}$	$i_{P,BM}$	0	$i_{TSS,BM}$
17	X_{TSS}	0	0	0	0	-1
18	X_{MeOH}	0	0	0	0	1
19	X_{MeP}	0	0	0	0	1

Table A2: ASM2d Stoichiometric Coefficients

symbol	Definition	Value	Unit
Typical conversion factors			
Nitrogen N			
i_{N,S_I}	N content of inert soluble COD S_I	0.01	$gN/gCOD$
i_{N,S_F}	N content of fermentable substrate S_F	0.03	$gN/gCOD$
i_{N,X_I}	N content of inert particulate COD X_I	0.02	$gN/gCOD$
i_{N,X_S}	N content of slowly biodegradable substrate X_S	0.04	$gN/gCOD$
$i_{N,BM}$	N content of biomass, X_H , X_{PAO} , X_{AUT}	0.07	$gN/gCOD$
Phosphorous P			
i_{P,S_I}	P content of inert soluble COD S_I	0.00	$gP/gCOD$
i_{P,S_F}	P content of fermentable substrate S_F	0.01	$gP/gCOD$
i_{P,X_I}	P content of inert particulate COD X_I	0.01	$gP/gCOD$
i_{P,X_S}	P content of slowly biodegradable substrate X_S	0.01	$gP/gCOD$
$i_{P,BM}$	P content of biomass, X_H , X_{PAO} , X_{AUT}	0.02	$gP/gCOD$
Total suspended solids TSS			
i_{TSS,X_I}	TSS to COD ratio for X_I	0.75	$gTSS/gCOD$
i_{TSS,X_S}	TSS to COD ratio for X_S	0.75	$gTSS/gCOD$
$i_{TSS,BM}$	TSS to COD ratio for biomass, X_H , X_{PAO} , X_{AUT}	0.90	$gTSS/gCOD$
Typical stoichiometric parameters			
Hydrolysis processes			
f_{S_I}	Production of S_I in hydrolysis	0.00	$gCOD/gCOD$
Heterotrophic organisms : X_H			
Y_H	Yield coefficient of heterotrophic biomass	0.625	$gCOD/gCOD$
f_{X_I}	Fraction of inert COD generated in biomass lysis	0.10	$gCOD/gCOD$
Phosphorous – accumulating organisms (PAO) : X_{PAO}			
Y_{PAO}	Yield coefficient (biomass /PHA)	0.625	$gCOD/gCOD$
Y_{PO_4}	PP requirement (PO_4 release) per PHA stored	0.4	$gP/gCOD$
Y_{PHA}	PHA requirement for PP storage	0.20	$gCOD/gP$
f_{X_I}	Fraction of inert COD generated in biomass lysis	0.10	$gCOD/gCOD$
Nitrifying organisms (autotrophic organisms) : X_{AUT}			
Y_A	Yield of autotrophic biomass	0.24	$gCOD/gN$
f_{X_I}	Fraction of inert COD generated in biomass lysis	0.10	$gCOD/gCOD$

Table A3: ASM2d Kinetic parameters

Par.	Definition	Value	Unit
Hydrolysis processes			
K_h	Hydrolysis rate constant	3.00	1/d
η_{NO3}	Anoxic hydrolysis reduction factor	0.60	-
η_{fe}	Anaerobic hydrolysis reduction factor	0.40	-
K_{O2}	Saturation/inhibition coefficient for oxygen	0.20	gO_2/m^3
K_{NO3}	Saturation/inhibition coefficient for nitrate	0.50	gN/m^3
K_X	Saturation/inhibition coefficient for particulate COD	0.10	gX_S/gX_H
Heterotrophic organisms : X_H			
μ_H	Maximum growth rate on substrate, heterotrophics	6.00	$gX_S/(gX_H * d)$
q_{fe}	Maximum rate for fermentation	3.00	$gS_F/(gX_H * d)$
η_{NO3}	Reduction factor for denitrification	0.80	-
b_H	Rate constant for lysis and decay, heterotrophs	0.40	1/d
K_{O2}	saturation/inhibition coefficient for oxygen	0.20	gO_2/m^3
K_F	Saturation coefficient for growth on SF	4.00	$gCOD/m^3$
K_{fe}	Saturation coefficient for fermentation of SF	4.00	$gCOD/m^3$
K_A	Saturation coefficient for growth on acetate SA	4.00	$gCOD/m^3$
K_{NO3}	Saturation/inhibition coefficient for nitrate	0.50	gN/m^3
K_{NH4}	Saturation coefficient for ammonium (nutrient)	0.05	gN/m^3
K_P	Saturation coefficient for phosphate (nutrient)	0.01	gP/m^3
K_{ALK}	Saturation coefficient for alkalinity (HCO ₃ ⁻)	0.10	$mole\ HCO_3^-/m^3$
Phosphorous – accumulating organisms (PAO) : X_{PAO}			
q_{PHA}	Rate constant for storage of XPHA (base XPP)	3.00	$gX_{PHO}/(gX_{PAO} * d)$
q_{PP}	Rate constant for storage of XPP	1.50	$gX_{PP}/(gX_{PAO} * d)$
μ_{PAO}	Maximum growth rate of PAO	1.00	1/d
η_{NO3}	reduction factor for anoxic activity	0.60	-
b_{PAO}	Rate for lysis of XPAO	0.20	1/d
b_{PP}	Rate for lysis of XPP	0.20	1/d
b_{PHA}	Rate for lysis of XPHA	0.20	1/d
K_{O2}	Saturation/inhibition coefficient, oxygen growth PAO	0.20	gO_2/m^3
K_{NO3}	Saturation coefficient for nitrate, SNO ₃ growth PAO	0.50	gN/m^3
K_A	Saturation coefficient for acetate, SA growth of PAO	4.00	$gCOD/m^3$
K_{NH4}	Saturation coefficient for ammonium growth of PAO	0.05	gN/m^3
K_{PS}	Saturation coefficient for phosphorous in storage of PP	0.20	gP/m^3
K_P	Saturation coefficient for phosphate, growth of PAO	0.01	gP/m^3
K_{ALK}	Saturation coefficient for alkalinity (HCO ₃ ⁻),	0.10	$mole\ HCO_3^-/m^3$
K_{PP}	Saturation coefficient for poly-phosphate	0.01	gX_{PP}/gX_{PAO}
K_{MAX}	Maximum ratio of XPP/XPAO	0.34	gX_{PP}/gX_{PAO}
K_{IPP}	Inhibition coefficient for PP storage	0.02	gX_{PP}/gX_{PAO}
K_{PHA}	Saturation coefficient or PHA	0.01	gX_{PHA}/gX_{PAO}

Nitrifying organisms (autotrophic organisms) : X_{AUT}			
μ_{AUT}	Maximum growth rate of XAUT	1.00	1/d
b_{AUT}	Decay rate of XAUT	0.15	1/d
K_{O_2}	Saturation coefficient for oxygen, aut. growth	0.50	gO_2/m^3
K_{NH_4}	Saturation coefficient for ammonium, aut. growth	1.00	gN/m^3
K_{ALK}	Saturation coefficient for alkalinity (HCO_3^-), aut. growth	0.50	$mole\ HCO_3^-/m^3$
K_P	Saturation coefficient for phosphorous, aut. growth	0.01	gP/m^3
Precipitation			
k_{PRE}	Rate constant for P precipitation	1.00	$m^3/(gFe(OH)_3 \cdot d)$
k_{RED}	Rate constant for redissolution	0.60	1/d
K_{ALK}	Saturation coefficient for alkalinity	0.50	$mole\ HCO_3^-/m^3$

Table A4: Process rate equations for ASM2d

j	Process component	Process rate equation ρ_j
Hydrolysis processes		
1	Aerobic hydrolysis	$K_h \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{X_S/X_H}{K_X + X_S/X_H} \cdot X_H$
2	Anoxic hydrolysis	$K_h \cdot \eta_{NO_3} \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{X_S/X_H}{K_X + X_S/X_H} \cdot X_H$
3	Anaerobic hydrolysis	$K_h \cdot \eta_{fe} \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{X_S/X_H}{K_X + X_S/X_H} \cdot X_H$
Heterotrophic organisms : X_H		
4	Growth on $S_F S_F$	$\mu_H \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_F}{K_F + S_F} \cdot \frac{S_F}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H * \rho_F$
5	Growth on $S_A S_A$	$\mu_H \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_A}{K_F + S_A} \cdot \frac{S_A}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H$
6	Denitrification with $S_F S_F$	$\mu_H \cdot \eta_{NO_3} \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{S_F}{K_F + S_F} \cdot \frac{S_F}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H$
7	Denitrification with S_A	$\mu_H \cdot \eta_{NO_3} \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{S_A}{K_A + S_A} \cdot \frac{S_A}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H$
8	fermentation of $S_F S_F$	$q_{fe} \cdot \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{S_F}{K_{fe} + S_F} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H$
9	Lysis	$b_H \cdot X_H$
Phosphorous – accumulating organisms (PAO) : X_{PAO}		
10	Storage of X_{PHA}	$q_{PHA} \cdot \frac{S_A}{K_A + S_A} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{PP}/X_{PAO}}{K_{PP} + X_{PP}/X_{PAO}} \cdot X_{PAO}$
11	Aerobic storage of X_{PP}	$q_{PP} \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{PO_4}}{K_{PS} + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot \frac{K_{MAX} - X_{PP}/X_{PAO}}{K_{IPP} + K_{MAX} - X_{PP}/X_{PAO}} \cdot X_{PAO} \rho_{PP}$
12	Anoxic storage of X_{PP}	$\rho_{11} \cdot \eta_{NO_3} \cdot \frac{K_{O_2}}{S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}$
13	Aerobic growth on X_{PHA}	$\mu_{PAO} \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot X_{PAO} * \rho_{PAO}$
14	Anoxic growth on X_{PP}	$\rho_{13} \cdot \eta_{NO_3} \cdot \frac{K_{O_2}}{S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}$
15	Lysis of PAO	$b_{PAO} \cdot X_{PAO} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}}$
16	Lysis of PP	$b_{PP} \cdot X_{PP} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}}$
17	Lysis of PHA	$b_{PHA} \cdot X_{PHA} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}}$
Nitrifying organisms (autotrophic organisms) : X_{AUT}		
18	Aerobic growth of X_{AUT}	$\mu_{AUT} \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_{AUT} * \rho_{AUT}$
19	Lysis	$b_{AUT} \cdot X_{AUT}$
Simultaneous precipitation of phosphorous with ferric hydroxide ($Fe(OH_3)$) :		
20	Precipitation	$k_{PRE} \cdot S_{PO_4} \cdot X_{MeOH}$
21	Redissolution	$k_{RED} \cdot X_{MeP} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}}$

Table A5: Stoichiometric matrix

Stoichiometric matrix for soluble components										
Process component		S_{O_2}	S_F	S_A	S_I	S_{NH_4}	S_{N_2}	S_{NO_3}	S_{PO_4}	S_{ALK}
		O_2	COD	COD	COD	N	N	N	P	mole
1	Aerobic hydrolysis		1.00			0.01				0.001
2	Anoxic hydrolysis		1.00			0.01				0.001
3	Anaerobic hydrolysis		1.00			0.01				0.001
Heterotrophic organisms : X_H										
4	Growth on S_F	-0.60	-1.60			-0.022			-0.004	-0.001
5	Growth on S_A	-0.06		-1.60		-0.07			-0.02	0.021
6	Denitrification with S_F		-1.60			-0.022	0.21	-0.21	-0.004	0.014
7	Denitrification with S_A			-1.60		-0.07	0.21	-0.21	-0.02	0.036
8	fermentation of S_F		-1	1		0.03			0.01	-0.014
9	Lysis					0.031			0.01	0.002
Phosphorous – accumulating organisms (PAO) : X_{PAO}										
10	Storage of PHA			-1					0.40	0.009
11	Aerobic storage of PP	-0.20							-1	0.016
12	Anoxic storage of PP						0.07	-0.07	-1	0.021
13	Aerobic growth	-0.60				-0.07			-0.02	-0.004
14	Anoxic growth					-0.07	0.21	-0.21	-0.02	0.011
15	Lysis of PAO					0.031			0.01	0.002
16	Lysis of PP								1	-0.016
17	Lysis of PHA			1						-0.016
Nitrifying organisms (autotrophic organisms) : X_{AUT}										
18	Aerobic growth	-18.0				-4.24		4.17	-0.02	-0.60
19	Lysis					0.031			0.01	0.002
Simultaneous precipitation of phosphorous with ferric hydroxide ($F_e(OH_3)$) :										
20	Precipitation								-1	0.048
21	Redissolution								1	-0.048

Stoichiometric matrix for soluble components											
Process component		X_I COD	X_S COD	X_H COD	X_{PAO} COD	X_{PP} P	X_{PHA} COD	X_A COD	X_{TSS} TSS	X_{MeOH} TSS	X_{MeP} TSS
1	Aerobic hydrolysis		-1.00						-0.75		
2	Anoxic hydrolysis		-1.00						-0.75		
3	Anaerobic hydrolysis		-1.00						-0.75		
Heterotrophic organisms : X_H											
4	Growth on S_F			1					0.90		
5	Growth on S_A			1					0.90		
6	Denitrification with S_F			1					0.90		
7	Denitrification with S_A			1					0.90		
8	fermentation of S_F										
9	Lysis	0.10	0.9	-1					-0.15		
Phosphorous – accumulating organisms (PAO) : X_{PAO}											
10	Storage of PHA					-0.40	1		-0.69		
11	Aerobic storage of PP					1	-0.20		3.11		
12	Anoxic storage of PP					1	-0.20		3.11		
13	Aerobic growth				1		-1.60		-0.06		
14	Anoxic growth				1		-1.60		-0.06		
15	Lysis of PAO	0.10	0.90		-1				-0.15		
16	Lysis of PP					-1			-3.23		
17	Lysis of PHA						-1		-0.60		
Nitrifying organisms (autotrophic organisms) : X_{AUT}											
18	Aerobic growth							1	0.90		
19	Lysis	0.10	0.90					-1	-0.15		
Simultaneous precipitation of phosphorous with ferric hydroxide ($F_e(OH_3)$) :											
20	Precipitation								1.42	-3.45	4.87
21	Redissolution								-1.42	3.45	-4.87

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